

(12)

(21) **2 547 755**

(22) 17.12.2004

(51) Int. Cl.:

G01N 33/58 (2006.01)

G01N 33/68 (2006.01)

(85) 30.05.2006

(86) PCT/EP04/014450

(87) WO05/059556

(30) 03029370.8 EP 19.12.2003

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(54) PROCÉDÉ D'ANALYSE DE MÉTABOLITES

(54) METHOD FOR ANALYSING METABOLITES

(57)

Described is a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled. This method may further comprise, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label. Furthermore described is a set of isotopically labeled metabolites obtainable by applying this method, as well as kits facilitating the application of this method and corresponding uses.



(12) **DEMANDE DE BREVET CANADIEN
CANADIAN PATENT APPLICATION**

(13) **A1**

(86) Date de dépôt PCT/PCT Filing Date: 2004/12/17
(87) Date publication PCT/PCT Publication Date: 2005/06/30
(85) Entrée phase nationale/National Entry: 2006/05/30
(86) N° demande PCT/PCT Application No.: EP 2004/014450
(87) N° publication PCT/PCT Publication No.: 2005/059556
(30) Priorité/Priority: 2003/12/19 (EP03029370.8)

(51) Cl.Int./Int.Cl. **G01N 33/58** (2006.01),
G01N 33/68 (2006.01)
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(57) Abrégé/Abstract:

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(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
30 June 2005 (30.06.2005)

PCT

(10) International Publication Number
WO 2005/059556 A1

(51) International Patent Classification⁷: **G01N 33/58**,
33/68

(21) International Application Number:
PCT/EP2004/014450

(22) International Filing Date:
17 December 2004 (17.12.2004)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
03029370.8 19 December 2003 (19.12.2003) EP

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(81) Designated States (unless otherwise indicated, for every
kind of national protection available): AE, AG, AL, AM,
AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN,
CX, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,
GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE,
KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG,
PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
ZW.

(84) Designated States (unless otherwise indicated, for every
kind of regional protection available): ARIPO (BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM,
ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM),
European (AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI,
FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO,
SE, SI, SK, TR), OAPI (BF, BJ, CF, CG, CI, CM, GA, GN,
GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

- with international search report
- before the expiration of the time limit for amending the
claims and to be republished in the event of receipt of
amendments

For two-letter codes and other abbreviations, refer to the "Guid-
ance Notes on Codes and Abbreviations" appearing at the begin-
ning of each regular issue of the PCT Gazette.

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WO 2005/059556 A1

DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

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THIS IS VOLUME 1 OF **4**
CONTAINING PAGES 1 TO **361**

NOTE: For additional volumes, please contact the Canadian Patent Office

NOM DU FICHIER / FILE NAME :

NOTE POUR LE TOME / VOLUME NOTE:

Method for analysing metabolites

The present application relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope label. This method may further comprise, prior to quantitatively determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label. The present invention also relates to sets of isotopically labeled metabolites obtainable by applying this method, as well as to kits facilitating the application of this method and to corresponding uses.

The present invention belongs to the field of metabolome analyses, also referred to as metabolic profiling, i.e. the quantitative analyses of metabolites in a biological sample with the aim to investigate the state of organisms in particular with respect to biochemical regulatory networks. In the prior art, the metabolome, besides the proteome, transcriptome and genome, has become the fourth cornerstone of biological systems analyses. Only metabolome analyses allows insight into nutrient use, biosynthetic capacity of organisms, signalling and communication mediated via low molecular weight compounds and biochemical adaptive processes. Therefore profiling analyses of relative changes of all metabolites within an organism is in demand for a true biological systems analysis.

Metabolome analyses are still in early development inter alia because, in contrast to genome, transcriptome and proteome analyses, metabolome analyses has to deal with a highly diverse range of chemicals covering substances from small molecular

weight volatiles up to polymers. Conventionally, different and specialised analytical platforms are used in order to analyse these different classes of compounds. Meanwhile, universally applicable analytical platforms have been developed for complex mixtures of compounds. These exploit molecular mass and chromatographic retention in so-called hyphenated technologies, like GC-MS, HPLC-MS or MALDI-TOF. Bench-top gas chromatography coupled to mass spectrometry (GC-MS) was the first technology platform proposed for large-scale metabolome analyses (Trethewey, 1999). The choice of this hyphenated technology took into regard the ideal combination of unsurpassed chromatographic separation with high selectivity, sensitivity, and dynamic range of quantitative mass detection. Moreover, both GC and electron impact ionisation (EI) mass spectrometry exhibit only minor matrix effects as compared to other MS techniques, as for example matrix assisted laser desorption/ionisation-time of flight (MALDI-TOF) (Guo, 2002) mass spectrometry or liquid chromatography coupled to mass detection (HPLC-MS) (Matuszewski, 2003). High reproducibility of the GC-MS analyses of metabolites, which routinely uses methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents, allowed metabolite profiling based on external quantification of respective methoxyamine (MX) and trimethylsilyl (TMS) derivatives (Fiehn, 2000a; Roessner, 2000; Roessner, 2001). The scope of metabolites covered is, however, limited (1) by the required volatility of metabolites or stable chemical derivatives of unstable metabolites, and (2) by the distribution of metabolite concentrations within each type of sample. The maximum sample load of any multi-parallel chemical analyses is determined by the predominating metabolites. GC-MS metabolite profiles have an enormous dynamic range of 4 to 5 orders of magnitude. The upper limit of quantification is set by the requirement for surplus chemical reagent and by peak deformation effects due to chromatographic overloading. Thus, biological matrices devoid of single predominant metabolites promise best potential for highly complex multi-parallel analyses (Fiehn, 2000a; Roessner, 2000).

Two main strategies are conceivable toward a more comprehensive metabolome analyses: (1) the choice of other analytical techniques which may supplement GC-MS analyses, and (2) the application of pre-fractionation and concentration techniques for the enrichment of trace compounds. However, both strategies are currently highly limited. Supplementary MS techniques, as for example MALDI-TOF-

MS or HPLC-MS, are subject to strong interferences, which result from the changing compositions of complex biological matrices. These so-called matrix effects may lead even to complete suppression of ionisation and response signal (Matuszewski, 2003; Guo, 2002). On the other hand, most pre-fractionation and concentration techniques result in high or highly variable losses of metabolites.

These drawbacks preventing the use of potentially more powerful MS techniques in metabolite profiling studies may at least in part be overcome by including internal standards into the metabolite analyses. Indeed, a thorough quantitative standardisation for as many as possible measured metabolites is required. This would make it possible to extend the scope of metabolite profiling to such techniques, because it would allow an exact quantification of the metabolite levels for which a standard is available. From investigations on metabolic fluxes, it is known that metabolites can be labeled in vivo with a stable isotope (Wittmann, 2002). However, flux analyses are generally confined to the investigation of very limited biochemical pathways and do not cover metabolites in the breadth as is normally required for metabolic profiling. Consequently, the substrate compounds which are used in such studies in order to label cells with a stable isotope are typically very specific to the particular biochemical pathway to be analysed. Their production is expensive because it requires specific and time-consuming chemical syntheses.

To summarize, a practicable approach for establishing a quantitative standard for use in metabolite profiling is not in sight in the prior art. This is mainly explained by the diversity of compound classes to which metabolites may belong and by the fact that most of the metabolites cannot be tagged after extraction as it is possible for the chemically uniform transcripts and proteins (see, e.g., Gygi, 1999).

Thus, the technical problem underlying the present invention is the provision of means and methods that allow it to improve metabolome analyses by establishing a reliable quantitative standard for as many as possible metabolites in order to broaden the scope of such analyses.

This technical problem is solved by the provision of the embodiments as characterized in the claims.

Accordingly, the present invention relates to a method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite, said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

The present invention is based on the experiments described in the appended Examples which show that it is possible to label substantially all possible metabolites in vivo. The proof that this principle works has been obtained by labeling yeast cells with U-¹³C-glucose. This work represents the keystone to comprehensive, fully quantitative metabolome profiling and will greatly facilitate future developments within this field. It solved the technical problem of standardisation by differential labeling of metabolites with isotopes. Similar to differential labeling of transcript samples by fluorescent probes or of protein samples by chemical tagging, it is possible in the method of the present invention to tag the metabolome by saturating in-vivo labeling with isotopes. This concept can be extensively exploited for a non-biased sampling of mass spectral metabolite tags (MSTs) and isotopomer ratio (ITR) metabolite profiling. In particular, isotope-saturated extracts produced by the method of the invention may be used as a multiplex mixture of internal standards, where each component of the resulting metabolite profiles will be quantified relative to the respective fully labeled isotopomer (see Example 4 and Figure 2). It is envisaged that these achievements, in particular the compilation of a first compendium of MSTs which, analogous to ESTs, allows qualitative assessment of the metabolome composition and the demonstration of fully quantitative ITR metabolite profiling, will greatly improve metabolome analyses.

In the prior art, isotope labeling studies are routine approaches used for metabolite flux analyses (Wittmann, 2002; Christensen (1999); Wiechert, 2001. These studies require isotopically labeled compounds, which are expensive and of limited availability. In a conventional flux experiment, a labeled compound is fed to

organisms, which are pre-grown on media with ambient isotope distribution (dos Santos, 2003; Lee, 1991) resulting in the labeling of a corresponding specific isotopically labeled metabolizable compound. However, flux studies differ from the method of the invention in that they generally involve partial labeling of the metabolites of a cell. This is explained by the fact that flux studies require partial, i.e. incomplete, labeling. By contrast, the method of the present invention achieves saturating labeling which means a labeling of the metabolites as complete as possible given the degree of labeling in the isotopically labeled metabolizable compound used to label the cell from which the biological sample for analyses is derived (for more detailed definitions see below).

One advantage of the present method is the fact that it introduces an isotopic label at the site which is ideal for metabolome analyses, namely the active biological sample. In prior art technologies, a differential label is often introduced only in the course of chemical analyses such as in the currently prevailing methods for quantitative proteome (Aebersold, 2003) and transcriptome (Duggan, 1999) analyses. These technologies for example involve isotope-coded protein-tagging techniques (Gygi, 1999) and two-colour labeling by fluorescent probes (Schena, 1995; Lockhart, 1996). However, labeling only after extracting the respective compounds from the cell may introduce a bias in the labeling result. Such artefacts are excluded in the method of the invention.

Apart from incorporation of label in the course of chemical analyses, there has been at least one approach to label proteins in vivo. Oda (Proc. Natl. Acad. Sci. USA 96 (1999), 6591-6596) describe whole cell-labeling for proteome analyses using the stable isotope ^{15}N . However, in vivo isotope labeling of the entire set of metabolites has not been reported in the prior art. In particular, by using ^{13}C -labeling of yeast cultures, the present invention demonstrates that combined mass spectral analyses of differentially labeled samples, especially ^{13}C -ITR profiles, can be generated. In particular, the experiments underlying the present invention surprisingly show that complete (i.e. saturating) labeling of metabolites could be achieved in yeast cells. The results obtained in the appended Examples are surprising because it could not have been excluded that carbon sources other than the isotopically labeled metabolizable compound (in the examples U- ^{13}C -glucose) which are present in the medium could have prevented an efficient broad isotope labeling of the metabolites.

It is almost impossible to avoid in the medium the presence of such other carbon sources like for instance essential nutrients, such as vitamins, or auxotrophic markers. The processing of these compounds in the cultured cells could have severely interfered with isotope labeling and thereby prevented the required saturating labeling. However, as is shown in the Example experiments, the lack of labeling in the cell due to the presence of the unlabeled carbon sources in the medium is greatly restricted to the compounds themselves or to direct metabolic products thereof (see Example 1). A mixing of label with unlabeled compounds essentially did not take place. This was surprising and means that in vivo labeling with isotopes can indeed be applied for achieving broad coverage of the metabolites with isotopic labeling.

Another surprising finding was that the presence of isotope label in the metabolites does not substantially influence the distribution of metabolite levels in the sample when it is compared with a metabolite profile obtained from a corresponding unlabeled sample (i.e. a sample, wherein the cells have been fed with nutrients in which the isotopes are present in the naturally occurring, i.e. ambient proportions). This is for example evident from the results depicted in Figure 2 and described in Example 4. This could not have been expected since it is known that enzymes may discriminate between isotopomers. For instance, such effects are described from plant physiology such as for RUBISCO, CO₂-fixation and phosphoenolpyruvate carboxylase (PEPC) (see, e.g., Le Roux-Swarthout, J. Plant Physiol. 157 (2000), 489-493) and from fungi, yeast or other microorganisms, e.g., for pyruvate decarboxylase (PDC), and the isoprenoid metabolism (see, e.g., Stivers, Biochem. 32 (1993), 13472-13482; Henn, Appl. Environ. Microbiol. 66 (2000) 4180-4186; Londry, Appl. Environ. Microbiol. 69 (2003), 2942-2949). Thus, it was reasonable to expect that, caused by isotope discrimination, the labeling of metabolites with isotopes would influence the distribution of metabolite levels in the biological sample. But, as it is shown herein, the isotopically labeled metabolites show a distribution that greatly corresponds to that obtained for unlabeled metabolites. This proves suitability of the method of the invention for standardizing metabolite analyses.

The experimental results summarized in the following show that the method of the invention may become an indispensable tool for the future development of metabolite profiling.

The present invention is herein exemplified in experiments using a *Saccharomyces cerevisiae* model which was subjected to saturating in vivo stable isotope labeling by growing on an exclusive ^{13}C -source (see, e.g., Figures 1 and 9). The in vivo labeling of metabolites in yeast generates isotopomer tags which could be differentially detected by mass spectrometry. When applied as internal quantitative standard, isotope-labeled compounds may facilitate a meaningful quantitative analyses if for example two samples, the one being saturatingly labeled and the other not being labeled (i.e. having ambient isotope abundances) are compared and the relative ratio between each isotopomer tag and the corresponding unlabeled metabolite is determined. Interestingly, this working principle may even facilitate those mass spectral technologies such as MALDI-TOF-MS which are prone to matrix suppression effects and high variability and which therefore hitherto were not applied for quantitative metabolite profiling analyses. An example of successfully using the method of the invention by applying MALDI-TOF-MS is presented herein (Example 9 and Figure 9). This means that the method described herein may allow to extend multi-parallel metabolite profiling in principle at least to all mass spectrometry-based technologies.

A further advantage of the method of the invention over conventional metabolome analyses is that it allows an immediate proof of the metabolic origin of any mass spectral tag which is detected in biological samples. While protein and mRNA sequence diversity provides information about the source species by the sequence information contained therein, the origin is not immanent in metabolite structure per se, except for the subset of species-specific secondary metabolites. However, as soon as a pair of labeled and non-labeled MSTs is found, chemical artefacts or laboratory contaminations can immediately be ruled out.

In addition, mass shifts allow a direct insight into the number of carbon atoms present within each compound or fragment. This property of the method of the invention increases the insight into the chemistry of those MSTs the chemical nature of which is unknown and may support the identification of MSTs by other techniques (Table 3).

In analogy to expressed sequence tags (ESTs), identified and non-identified MSTs may be used as a highly useful tool to characterise the metabolome of any biological sample. Again in analogy to tools for sequence comparison, MSTs can easily be

identified by matching of mass spectral fragmentation and chromatographic retention. Furthermore, clustering technologies allow a meaningful classification of MSTs (Figure 4) (Wagner, 2003).

As a further advantageous property, the method of the invention allows a fast investigation of the precision of analytical methods which are being developed for metabolite profiling. In addition, it makes quantitatively standardized metabolome analyses accessible to biological samples which are obtained by pre-purification and enrichment of fractions of the total metabolite extract taken from a biological sample, for instance in order to detect trace metabolites. In the prior art, such samples fall below the detection limits of conventional GC-MS profiling. The possibility of the method of the invention to quantitatively determine minor amounts of metabolites facilitates to conduct metabolite co-response analyses which may provide direct information about quantitative metabolite interactions in biological systems. Such interactions may be expected based on theoretical considerations (Steuer, 2003). Observed metabolite co-responses may be uncoupled or may follow linear functions. Metabolite co-response may be either constitutive or conditional with respect to the set of experiments under investigation. In Example 8, metabolite co-response analyses applying the method of the invention are described. Accordingly, metabolite co-responses may best be discovered and judged by a set of different distance measures, among which the Euclidian distance is least indicative (Figure 6). Metabolite interactions may reflect canonical pathway definitions (Figure 7), but may also allow to discover cross-pathway interactions (Figure 8). Investigations into these interactions are highly valuable, because they can provide insights into common mechanisms of metabolic control. However, to date, such analyses are restricted due to the limited coverage of metabolome data. Based on the extension of metabolite data mining that is now possible by applying the method of the invention, for instance because of the possibility to exploit MALDI-TOF for quantitative determination of metabolite levels on a broad scale, it is conceivable that the present invention will further the development of quantitative metabolome analyses, in particular towards trace compounds and general co-factors.

As it is explained above, the present invention belongs to the field of the metabolic profiling or metabolome analyses. This means that the method of the invention is of use for quantitatively determining one or more metabolites in a biological sample.

The term "quantitative determining" refers to the determination of the relative or absolute amount of each analyzed metabolite in the sample. Generally, such a determination leads to a so-called metabolite profile pertaining to the respective biological sample. Such metabolite profiling approaches have been carried out in many laboratories and therefore belong to the prior art.

Since isotopic labeling is applied in the method of the invention, it is necessary that the technique used to quantitatively determine the metabolites resolves isotopic mass differences as they may occur within one metabolite. Compounds that differ from one another only by one or more isotopes incorporated into the chemical structure are generally referred to as "isotopomers". The technique used to detect the metabolites must therefore be capable of discriminating between two compounds that differ in their mass by as little as one relative atomic mass. Corresponding techniques are known to the skilled practitioner and described in the literature. They involve different kinds of mass spectrometry or NMR, as is described in further detail further below.

The term "isotopic labeling" is to be understood to refer to compounds that are labeled with an isotope that is not the main isotope of the element of said isotope. "Labeled" means in this context to have a significantly and, for detection purposes, usefully increased proportion of the label-isotope as compared to the abundance of said isotope occurring in nature, preferably the proportion of the label-isotope is increased to at least 80%, more preferably to at least 90% and even more preferably to at least 95% and most preferred to at least 99% of the total of all isotopes of the respective element. The term "isotopic labeling" furthermore preferentially refers to compounds in which the label-isotope is present in the above-mentioned proportion at each possible position within the chemical structure of the compound. However, partial labeling of compounds may also be of use in the context of the present invention. Such applications require that means of correction for the proportion of residual non-labeled isotopomers are applied. In this case, labeling needs to be saturating, i.e. the proportions of isotopomers for each metabolite needs to be constant in the labeled sample, so that the isotopomer proportions can be

determined in a control experiment and used for mathematical correction of the metabolite profiling results. Preferably, the isotopically labeled metabolizable compound used in order to label the cell contains of the respective element only the label-isotope (in the proportion that is technically feasible) as it is the case with U- ^{13}C -glucose where all six carbon atoms are the ^{13}C isotope.

The method of the present invention is characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

It is a critical feature of the method of the invention that the metabolites are saturated with the isotopic labeling. "Saturated" (or "saturating labeling") means that the metabolites in the cell or the biological sample derived therefrom contain an amount of isotope label that substantially corresponds to the amount of label in the metabolizable compound taken up by the cell in order to label it, and that substantially all of the metabolites to be analyzed contain the isotope label. In particular, "saturating labeling" refers to an amount of labeling of the metabolites to be analyzed so that these metabolites overall contain at least 50%, preferably at least 70%, more preferably at least 80%, still more preferably at least 90% and most preferably at least 95% of the amount of isotopic label as present in the isotopically labeled metabolizable compound. The term "substantially all of the metabolites to be analyzed contain the isotope label" means that at least 70%, preferably at least 80%, more preferably at least 90%, still more preferably at least 95% and most preferably at least 98% of the metabolites to be analyzed are labeled, i.e. differ by at least one relative atomic mass from the corresponding unlabeled counterpart. Preferably, substantially all of the metabolites to be analyzed contain the isotope label if at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites of the biological sample to be analyzed contain the isotopic label.

Exceptions to the labeling to saturation may be tolerated, however, should be taken into account when analysing the metabolite data obtained. Non-labeled metabolites may be present in the biological sample when, in addition to the isotopically labeled metabolizable compound, other compounds, for example essential nutrients like

metabolizable compound, other compounds, for example essential nutrients like vitamins or auxotrophy markers, have been provided to the cell via the culture medium and these compounds do not contain the isotope label. Therefore, it may happen that cells which are labeled to saturation contain unlabeled metabolites which are these other compounds or metabolic products thereof.

The number and selection of metabolites analyzed in the method of the invention depends on the goal to be achieved by carrying out the method of the invention. It is typical for metabolic profiling like the method of the invention to aim at quantitatively determining an as large as possible subset of metabolites in order to obtain as much as possible metabolite data. Here, the possibility to label in principle each metabolite by the method of the invention is a big advantage over prior art approaches because it provides a quantitative standard for each metabolite to be analyzed.

Accordingly, in a preferred embodiment of the method of the invention, at least 20, more preferably at least 50, still more preferably at least 100, even more preferably at least 150 and most preferably at least 200 or even at least 300 metabolites are quantitatively determined.

The term "metabolite" refers to any substance within a cell or produced by a cell, including secreted substances, which can be quantitatively determined by applying the method of the invention, that is for which suitable techniques for determining the amount are available. Preferably, these substances are not macromolecules (i.e. biopolymers) such as DNA, RNA or proteins. Particularly preferred are metabolites with a low molecular weight preferably the metabolites have a molecular weight of not more than 4000 Da, preferably not more than 2000 Da, more preferably not more than 1000 Da. Typically, the metabolites to be analyzed may belong to the following, non-limiting list of compounds: carbohydrates (e.g. sugars, oligo- and polysaccharides such as polyglucans as for example starch or polyfructans), sugar alcohols, amines, polyamines, amino alcohols, aliphatics, aliphatic alcohols, amino acids, lipids, fatty acids, fatty alcohols, organic acids, organic phosphates, organic ions, other inorganic ions bound to metabolites, nucleosides, nucleotides, sugar nucleotides, purines, pyrimidines, such as adenine and uracil, sterols, terpenes, terpenoids, flavons and flavonoids, glucosides, carotenes, carotenoids, cofactors,

ascorbate, tocopherol, vitamins, polyols, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.

As is evident from the appended Examples, the method of the invention also involves analysing metabolites of which the chemical nature is unknown. However, metabolites (herein also referred to as "mass spectral metabolite tags" or "MSTs") of unknown chemical nature may nevertheless provide informative data on the biological sample analysed. It is clear that, if a metabolite of unknown chemical nature is revealed by carrying out the method of the invention to have an interesting property or diagnostic value or characteristic behaviour, this metabolite may be further characterized by applying suitable analytical methods known in the art.

In a particularly preferred embodiment, the method of the invention refers to the quantitative determination of metabolites comprising sugars, sugar alcohols, organic acids, amino acids, fatty acids, vitamins, sterols, organic phosphates, polyamines, polyols, nucleosides, purines, pyrimidines, adenine, uracil, organic amines and amides such as ethanol amine and urea and/or heterocyclic compounds such as nicotinic acid.

The isotope used for in vivo labeling in connection with the present invention may be selected among available isotopes that may be suitable for applying the method of the invention. As a preferred selection, a skilled person may use an isotope for which corresponding isotopically labeled metabolizable compounds are available, in particular commercially available. As a further preferred choice, isotopes for use in the method of the invention should be such that they do not harm viability of the cells from which the biological sample for analyses is taken or that they do not interfere with the metabolism such as by influencing the activity of metabolic enzymes. In this regard, it is thus preferred to use stable isotopes rather than radioactive ones. As a further aspect, one should take into account that elements such as carbon or hydrogen are preferred over elements that are present in metabolites more rarely in order to cover the metabolites of a cell by in vivo labeling as completely as possible. Particularly preferred isotopes are ^{13}C , ^{15}N , ^{18}O and ^2H , with particular preference of ^{13}C .

The label-isotope is incorporated into the cells from which the biological sample for analyses is taken by maintaining the cell under conditions allowing the uptake of said compound. This means that the compound should be one that is readily taken up by the cells and that is also readily metabolized so that it is ensured that saturation with the isotopic label can be achieved. Depending on the kind of cells or organism to be labeled, the label may for example be provided by feeding cultured cells such as yeast cells or mammalian cells with a nutrient, e.g. a carbon source if the label is ^{13}C . If the cells to be labeled are within a multicellular organism, the label may be incorporated by subjecting the labeled metabolizable compound through the substrate (e.g. the water) if it is a plant or by injecting the labeled compound into it if the organism is an animal, for instance a vertebrate, in particular a mammal.

As the isotopically labeled metabolizable compound, substances should be used that provide for an effective uptake of the label by the cell. Preferably, the compound may be totally labeled with the isotope (i.e. no atom of the respective element in the compound is of another isotope than the label-isotope). Corresponding labeled compounds may be available from commercial suppliers such as those mentioned in the Examples. Particularly preferred isotopically labeled metabolizable compounds are $\text{U-}^{13}\text{C}$ -glucose, $^2\text{H}_2\text{O}$, H_2^{18}O , $\text{U-}^{13}\text{C}$ acidic acid, ^{13}C carbonate and ^{13}C carbonic acid.

The term "biological sample" encompasses any amount of material comprising cells or derived from a cell that is susceptible to the method of the invention. In the present context, the term "cell" refers to any conceivable living entity that is capable of being in vivo-labeled according to the teachings of the present invention. Accordingly, the method may be applied to any type of cell, prokaryotic or eukaryotic cells, viral particles, wild-type or transformed, transduced or fused cells, or derivatives thereof such as membrane preparations, liposomes and the like. The cells may furthermore be part of a tissue, an organ or a complete organism such as a plant or an animal. The cells may be in a naturally occurring form or in a man-made form such as in a cultured form, e.g. cell culture, protoplast culture, tissue culture or the like.

The term "derived" used in connection with characterizing the biological sample means any kind of measures a skilled person may apply in order to modify the labeled cells or the direct environment of the cells, wherein the "direct environment"

is characterized by the presence of at least one metabolite produced by the cells, in order to prepare a sample for use in quantitatively determining the metabolites contained therein by applying the method of the invention. Such measures may for example involve typical sample preparation or extraction techniques common to those skilled in the art. The direct environment may for example be the extracellular space around a cell, the apoplast, the cell wall, the interstitial space or the culture medium. Furthermore, the biological sample derived from a cell may be a certain part of the cell, for example certain cellular compartments such as plastids, mitochondria, the nucleus, vacuoles etc. In a preferred embodiment of the present invention, the biological sample comprises yeast cells or plant cells.

A "biological sample" in the context of the present invention can for instance be fresh material such as a tissue explant, a body fluid or an aliquot from a bacterial or cell culture, preferably deprived of the culture medium, that may be directly subjected to extraction. On the other hand, samples may also be stored for a certain time period, preferably in a form that prevents degradation of the metabolites in the sample. For this purpose, the sample may be frozen, for instance in liquid nitrogen, or lyophilized. The samples may be prepared according to methods known to the person skilled in the art and as described in the literature. In particular, the preparation should be carried out in a way suitable to the respective detection technique applied. Furthermore, care should be taken that the respective compounds to be analyzed are not degraded during the extraction process. Biological samples for metabolite analyses may for example be prepared according to procedures described in Roessner (2000).

In a further preferred embodiment, the method of the invention further comprises fractionating or purifying the biological sample so that the sample contains a subset of the metabolites contained in the cell from which the sample is derived.

By this additional fractionation and/or purification step, it is for example possible to select low abundant metabolites out of the whole pool of metabolites whereby, without this step, these metabolites might not be detectable for example because their signals are superimposed with strong signals of highly abundant metabolites. In prior art metabolite profiling methods, such a fractionation or purification would cause the loss of the quantitative relationship to other metabolites which would render the

quantification of low abundant metabolites nearly impossible. This problem has been overcome by the present invention since the isotopically labeled metabolites serve as a quantitative standard that may be co-fractionated/-purified with the non-labeled metabolites.

The fractionation and/or purification may be carried out according to standard procedures known in the art. It is clear that preferably procedures should be used that do not or at least only to a low tolerable degree change the distribution of the metabolites in the sample.

The quantitative determination of metabolites in a biological sample may be carried out by any known suitable method that can resolve mass differences within one metabolite. This may involve various nuclear magnet resonance (NMR) and mass spectrometry (MS) techniques that are known to a person skilled in the art, whereby mass spectrometry is preferred in the context of the present invention. Different suitable NMR and MS techniques are for instance described in Wittmann (Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) and Szyperski (Q. Rev. Biophys. 31 (1998), 41-106). Preferred set ups for MS techniques for use in the present invention involve the combination of MS with gas chromatography (GC) as it is routinely used in state-of-the-art metabolite analyses, such as GC-MS described in the appended Examples.

In cases of ambiguous fragment interpretation, analyses using GC-MS-MS or corresponding MS tandem arrangements may support the identification of isotopomer fragment pairs. For example, GC-MS systems supplied with ion trap technology allow the selection of individual primary fragments and subsequent secondary mass spectral fragmentation (Birkemeyer, 2003; Mueller, 2002). These MS-MS mass spectral fingerprints may allow an unequivocal identification of corresponding primary ions.

The determination of the amount of metabolites of interest can be done according to well-known techniques known in the prior art and familiar to the person skilled in the art. Preferably, techniques are applied that allow the identification and quantification in one step and, advantageously, are suited to record the respective metabolites contained in the sample in a comprehensive manner.

Further methods for quantitatively determining the metabolites for use in accordance in the present invention include liquid chromatography/mass spectrometry (LC/MS), the use of radioactivity in connection with suitable methods known to the skilled person, thin layer chromatography (TLC), capillary electrophoresis (CE), direct injection MS, flow injection MS, MS/MS, MS/MS/MS, and further combinations of MS steps (MS_n), fourier transform ion mass spectrometry (FT/MS), gel permeation chromatography (GPC), TLC, CE, HPLC, GPC, any other chromatographic or electrophoretic technique or any mass spectrometric technique which is hyphenated in-line or off-line to mass spectrometry. If appropriate, any of the above methods may be combined.

An exemplary non-biased analyses is described in Fiehn (2000b). In this study, of different plant mutants, 326 distinct compounds (ranging from primary polar metabolites to sterols) were detected and relatively quantified, including both identified and non-identified compounds, by applying GC/MS analyses. Another example of a GC/MS analyses that can be applied in the method of the invention has been described by Roessner (2001), where it was used for comprehensively studying the metabolism in potato tubers.

In a particularly preferred embodiment of the method of the invention, the mass spectrometry used is matrix-assisted laser desorption ionisation/time-of-flight (MALDI-TOF) mass spectrometry.

This embodiment makes use of the surprising finding that the saturating in vivo labeling achieved by the method of the invention makes it possible to obtain quantitative metabolite profile data.

It is furthermore preferred that the method of the invention as described hereinabove involves that the metabolites are chromatographically separated prior to quantitative determination.

This preferred embodiment refers to the chromatographic separation which has already been described above by referring to the particularly preferred example of using gas chromatography in settings such as GC-MS or GC-MS-MS. Other suitable chromatography methods such as HPLC, RP-HPLC, ion-exchange HPLC, GPC, capillary electrophoresis, electrophoresis, TLC, chip-base micro-fluidic separation,

affinity-interaction chromatography using antibodies or other ligand-specific binding domains may also be used in this regard.

In another preferred embodiment, the method of the invention further comprises the step of introducing external standards for one or more of the quantitatively determined metabolites.

The introduction of external standards or standard dilution series allows the determination of metabolite concentrations in absolute terms. By contrast, embodiments of the method of the invention in which no external standards or standard dilution series are applied allow the exact quantification in relative terms, i.e. concentration changes observed relative to reference quantities as observed in experimental control samples. The introduction of external standards and the provision of such standards may be carried out as described in the literature and as is known by the person skilled in the art.

As has been mentioned above, the method of the invention includes the quantitative determination of metabolites the chemical nature of which is yet unknown. Accordingly, in a preferred embodiment, this method further comprises the step of identifying one or more of the metabolites which are quantitatively determined.

This identification may be carried out by analytical methods known to the skilled practitioner and described in the literature.

In a particularly preferred embodiment, this identification comprises identification by secondary fragmentation.

Secondary fragmentation techniques may be carried out by methods known in the prior art, in particular by GC-MS-MS or other MSⁿ techniques. Separate recording and subsequent comparison of chemical intermediates from MS-MS fragmentation pathways of, e.g., ¹³C isotopomer pairs is highly facilitated by providing the number of carbon atoms present within each observed MS-MS fragment.

In an especially preferred form of this embodiment, identification of the metabolites comprises electron impact ionisation, MS-MS technology and/or post source decay analyses of molecular ions or fragments.

Such techniques are known to a person skilled in the art. In particular, post source decay analyses may be carried out as is described in Example 9 using NADH detection as an example.

In a further preferred embodiment, the method of the invention as described above may be carried out in such a way that the cell to be labeled has been maintained under conditions additionally allowing the uptake of an isotopically unlabeled metabolizable compound and said compound and/or metabolic products thereof are quantitatively determined. Preferably, the uptake of the unlabeled compound takes place when the cell is already saturated with the isotopic label.

Preferably, this embodiment involves comparing the amount determined for the isotopically unlabeled metabolizable compound and/or said metabolic products thereof with the amount obtained by carrying out said method correspondingly, but without the uptake of said unlabeled metabolizable compound.

The present preferred embodiment relates to an application of the present invention which is also referred to as "inverse labeling". This term refers to an inversion of conventional flux studies (see, e.g., Wittmann, Adv. Biochem. Engin. Biotechnol. 74 (2002), 39-64) in which a labeled metabolite is added to a cell and its fate is traced in order to analyse metabolic pathways. The present preferred embodiment of the invention appears to be feasible because of the high similarity of metabolite profiles from ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast cultures (Figure 2 A, B). Moreover, in Example 2, a corresponding experiment is described in which L-lysine was added in unlabeled form to the culture medium after the yeast cells reached saturated ^{13}C -labeling. In a further experiment, the enrichment of the non-labeled trace compound nicotinic acid and the incorporation of this moiety into NAD(H) within a ^{13}C -saturated yeast metabolome was shown (Example 9).

The present embodiment allows it to achieve results similar to those obtained in conventional flux studies. It allows to utilize the relatively inexpensive supply of substances with ambient $\delta^{13}\text{C}$ composition for biochemical pathway elucidation within the background of a ^{13}C -saturated metabolome. But it has the advantage that the specific metabolite the metabolization of which shall be analysed does not need to be provided in labeled form, which often is considerably expensive. Rather, in the method according to the present embodiment, the metabolite to be investigated can

be used in the cheaper unlabeled form. A further advantage is the increased versatility of this approach as compared to conventional flux studies since virtually every possible metabolite can be tested for or even more than one metabolite, without being dependent on the availability of the metabolite(s) in labeled form.

In a further preferred embodiment of the above-described method of the invention, one or more proteins and/or transcripts in said sample(s) is/are quantitatively determined and analysed, in addition to metabolites.

This embodiment refers to one of the main aspects in systems biology which aims at combining metabolome data with data obtained from transcriptome and/or proteome analyses in order to obtain a comprehensive picture of regulatory mechanisms in biological systems. In this context, it is evident that the method of the present invention may be combined with methods that quantitatively determine transcripts and/or proteins from the same biological system, in particular organism or cells, of which the metabolites are quantitatively analysed in accordance with the method of the invention. Transcriptome and proteome analyses as well as mathematical evaluation and correlation analyses of the data may be conducted by methods described in the prior art. It is contemplated that, preferably, the transcriptome and/or proteome analyses conducted in combination with the metabolome analyses according to the present invention may also benefit from the advantages of in vivo labeling. Thus, if the quantitative determination of transcripts or proteins is done by suitable techniques such as mass spectrometry the transcripts or proteins may be isotopically labeled just as the metabolites and thereby also be used as a quantitative standard.

It is particularly preferred that the preferred embodiment is carried out in such a manner that said metabolites and proteins and/or transcripts are each determined from the same biological sample.

This particularly preferred embodiment is based on a technology described in WO 03/058238 and in Fiehn (Eur. J. Biochem. 270 (2003), 579-588). The method described therein provides data useful for quantitatively analyzing metabolites, proteins and/or RNA in a biological source material, whereby said analyses involves suitable statistical evaluation and correlation analyses on the data obtained. In this

method, extracting, identifying and quantifying of at least two compound classes of the group consisting of metabolites, proteins and RNA are each determined from one sample. Accordingly, in the present particularly preferred embodiment, the sample preparation in order to quantitatively determine metabolites and proteins and/or transcripts is carried out by applying the corresponding teachings of WO 03/058238. Thereby, it is especially preferred that (i) the metabolites are extracted from the sample with at least one solvent or mixture of solvents; and (ii) the RNA is extracted from the remainder of the sample after step (i). Thereby, it is a further option that metabolites may additionally be extracted from the yet undissolved remaining cellular material contained in the sample after step (ii). Preferably, extraction is carried out by using a mixture of solvents that comprises at least one highly polar solvent, at least one less polar solvent and at least one lipophilic solvent, advantageously a mixture of solvents comprising water, methanol and chloroform. More preferably, this mixture of solvents contains water, methanol and chloroform in the approximate proportion by volume of 1: 2.5: 1. Advantageously, the extraction in step (i) is carried out at a temperature between -60°C and +4°C.

As a further preferred embodiment of the present invention, the method as described hereinabove further comprises, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label.

Preferably, the second biological sample is not isotopically labeled.

By this preferred embodiment, the method facilitates the quantification of metabolite data which hitherto was only possible by using external metabolite samples as quantitative standards. Here, the in vivo labeled metabolites present the quantitative standard for the metabolites of the second biological sample. This allows the correlation analyses of a wide set of metabolites of two biological samples which correspond to two different phenotypic and/or genotypic states of the cells from which the biological samples are derived.

Accordingly, in a specifically preferred embodiment, the first and the second biological sample correspond to different phenotypic and/or genotypic states of the cells comprised in the samples or from which the samples are derived.

By applying this embodiment of the method of the invention, it is possible to find correlations between the difference in the phenotypic and/or genotypic state and changes in the metabolite profile for instance by performing metabolite co-response analyses.

The term "phenotypic state" refers to differences in the phenotype of the cell under investigation or the organism in which it resides. "Phenotype" means any kind of feature that can be detected and which is not a feature of the genome. Such phenotypic states may for example be visually identifiable such as a morphological or anatomical difference like they can be observed at different developmental stages. Phenotypic states may likewise manifest themselves by the composition of chemical compounds or the occurrence of a disease. Thus, the phenotypic states may for instance be a healthy state in comparison to one or more pathogenic states, different stages of a pathogenicity or an uninfected versus one or more infected organisms.

The term "genotypic state" reflects differences in the genome of the cells under investigation. Thus, if the samples are taken from different genotypic states of a cell, the term "cell" specifically refers to cells according to the definition given above which belong to the same taxonomic unit, but which differ in at least one genetic trait. Specifically, the "taxonomic unit" is a genus, preferably a species, and more preferably an even lower taxonomic rank such as a race, variety, cultivar, strain, isolate, population or the like. Most preferably, the taxonomic rank is an isogenic line with variance in only a limited number, preferably three, more preferably two genetic traits and most preferably one genetic trait, whereby "genetic trait" refers to a chromosomal region, a gene locus or, as it is preferred, to a gene. Typically, differences in the genotypic state can be differences between a wild-type organism and one or more corresponding mutant or transgenic organisms or between different mutant or transgenic organisms. A certain genotypic state may be stable or transient as is the case with transduced or transfected cells, for instance containing a plasmid, phage or viral vector. Advantageously, organisms of different genotypic state are analyzed when they are in the same developmental stage.

It is immediately clear that the terms "phenotypic" and "genotypic" states may overlap. In particular, normally a genotypic state, if the differing genetic trait(s) is/are expressed in the organism, lead(s) to a difference in the phenotype.

According to the above explanations, in a preferred embodiment of the method of the invention, the different phenotypic and/or genotypic states are different developmental stages, environments, nutritional supplies, taxonomic units, wild-type and mutant or transgenic genomes, infected and uninfected states, diseased and healthy states or different stages of a pathogenicity.

In a further preferred embodiment of the method of the invention as described hereinabove, said analysing further involves suitable statistical evaluation and correlation analyses of the data obtained and, optionally, network analyses.

This refers to any mathematical analyses method that is suited to further process the quantitative data provided by the method of the invention. This data represents the amount of the analyzed metabolites present in each sample either in absolute terms (e.g. weight or moles per weight sample) or in relative terms (i.e. normalized to a certain reference quantity).

Quantitative analyses involves suitable statistical evaluation and correlation analyses. The former includes normalization to the total content of the respective compounds, correction of background levels and the combination of the data sets obtained from different experiments (if more than one sample is analysed) into a single data sheet. Corresponding mathematical methods and computer programs are known to the skilled practitioner. Examples include SAS, SPSS and systatR. As the next step, the statistically pre-treated data may be subjected to a pairwise correlation analyses. Here series of pairs of data points from the analyzed compounds are looked at for correlation, whether positive or negative, for instance using Pearson's correlation coefficient.

In a preferred embodiment, the quantitative analyses referred to in the method of the invention furthermore involves network analyses. Network analyses aims at finding out higher order interplays of multiple factors on the basis of pairwise correlation data. If, according to one of the above-described preferred embodiments, metabolites and transcripts and/or proteins are quantitatively determined, for the obtained several

data sets, preferably each obtained from one sample, correlations between metabolites and proteins and/or transcripts as well as within these classes of compounds can be analyzed in order to derive information about the network regulation of biological systems, e.g. upon genetic or environmental perturbation. A comprehensive overview of methods for quantitatively analyzing data obtained according to the method of the invention including principle component analyses, "snapshot analyses", Pearson correlation analyses, mutual information and network analyses can be found in Fiehn (2001).

In a further aspect, the present invention relates to a set of isotopically labeled metabolites obtainable from a sample which comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

The present invention also relates to such cells which can be cells as described above in connection with the method of the invention.

As is explained hereinbefore, the isotopically labeled metabolites obtained from a biological sample in accordance with the method of the present invention may be used as a quantitative standard for the quantitative determination of the metabolites of a second biological sample. Thus, a set of these labeled metabolites is also an object of the present invention. Preferably, this set can be used to standardize results of a metabolome analyses conducted with the same species of cells as that from which the set of metabolites is obtained. However, it is also feasible that this set may be of use to standardize metabolite data obtained from a different species. This would generally require that metabolites of the set are identical with metabolites of the second biological sample. Identity can be determined or confirmed by using methods known in the art and described herein. For instance, the in vivo isotopically labeled metabolites obtained from yeast may be used as a quantitative standard for metabolites of plant cells since, for a considerable subset of each of these metabolites, the metabolites overlap such as the metabolites of the primary metabolic pathways.

As a further use of the set of isotopically labeled metabolites of the invention, or corresponding cells containing them, it is envisaged that the set or the cells can be

used as a qualitative standard in order to identify metabolites from a second, unlabeled biological sample.

The set of metabolites may be prepared in accordance with the above explanations for carrying out the method of the invention. For the purposes of storing and transporting that set, corresponding methods may be applied which are suitable in order to ensure that degradation of each kind of metabolite contained therein is at least minimized to a tolerable degree and which are known to a person skilled in the art.

In a further embodiment, the present invention refers to the use of the set of isotopically labeled metabolites mentioned above as a quantitative standard for determining the amount of one or more metabolites in a biological sample.

Furthermore, the present invention relates to a kit comprising an isotopically labeled metabolizable compound and a manual for use in carrying out the method of the invention or the set of isotopically labeled metabolites described above.

The components of the kit of the invention may be packaged in containers such as vials in a storable and transportable form. If appropriate, one or more of said components may be packaged in one and the same container.

Additionally, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for labeling the metabolites in said cell in a saturating manner.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

The present invention also relates to the use of an isotopically labeled compound that can be metabolized by a cell for the quantitative determination of metabolites in a biological sample comprising or being derived from said cell.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

Likewise, the present invention relates to the use of an isotopically labeled compound that can be metabolized by a cell for analysing the metabolite profile of a biological sample comprising or being derived from said cell.

Such uses may be carried out in accordance with the above-outlined explanations for the method of the invention.

These and other embodiments are disclosed and encompassed by the description and examples of the present invention. All of the publications, patents and patent applications referred to in the specification in order to illustrate the invention are hereby incorporated by the reference in their entirety. Further literature concerning any one of the methods, uses and compounds to be employed in accordance with the present invention may be retrieved from public libraries, using for example electronic devices. For example the public database "Medline" may be utilized which is available on the Internet, for example under <http://www.ncbi.nlm.nih.gov/PubMed/medline.html>. Further databases and addresses, such as <http://www.ncbi.nlm.nih.gov/>, <http://www.infobiogen.fr/>, http://www.fmi.ch/biology/research_tools.html, <http://www.tigr.org/>, are known to the person skilled in the art and can also be obtained using, e.g., <http://www.google.de>. An overview of patent information in biotechnology and a survey of relevant sources of patent information useful for retrospective searching and for current awareness is given in Berks, TIBTECH 12 (1994), 352-364.

Furthermore, the term "and/or" when occurring herein includes the meaning of "and", "or" and "all or any other combination of the elements connected by said term".

The present invention is further described by reference to the following non-limiting figures, tables and examples.

The Figures and the Tables show:

Figure 1 shows the results of head-to-tail analyses of electron impact ionisation mass spectra of yeast metabolites extracted from GC-MS metabolite profiles.

The yeast metabolites succinic acid, glycine and glutamic acid were trimethylsilylated prior to GC analyses. The number of silylated functional groups and the magnification factor of the high molecular mass range is indicated. Head-to-tail mass spectra are from separate GC-MS analyses of ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast extracts. Insets to the right show the M^+ and $[\text{M}-15]^+$ fragment ranges of combined ^{13}C -isotopomer ratio (ITR) metabolite profiles. The isotopomer $[\text{M}-15]^+$ fragment pairs of succinic acid (2TMS), glycine (3TMS), and glutamic acid (3TMS) are M/Z 247_251, M/Z 276_278, and M/Z 348_353. Glutamic acid (3TMS) exhibited abundant molecular ions, M^+ , M/Z 363_368.

Figure 2 depicts a comparison of ITR metabolite profiling (A, C) and conventional metabolite profiling (B,D).

Selected ion responses of ^{12}C - and ^{13}C -isotopomer fragment pairs, which represent the same substance from ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast extracts (A, B), and fragments which represent the same isotopomer in two different experiments (Exp1 and Exp2) from either the ambient $\delta^{13}\text{C}$ - or ^{13}C -saturated yeast culture (C, D) are plotted. ITR was performed in two GC-MS analyses (06, 10), whereas four GC-MS analyses were required for conventional metabolite profiling (ambient $\delta^{13}\text{C}$: 04, 08; ^{13}C -saturated: 05, 09). Pearson's linear correlation coefficients (r) and average coefficients of variation (cf) are shown in the insets.

Figure 3 represents a GC-TOF-MS metabolite profile of yeast strain BY4741.

Ticks below the total ion current trace of the main profile indicate the automated deconvolution of mass spectral components with $\text{S/N} \geq 100$ which were performed by Pegasus chromatography data processing software. The inset shows selected ion traces of deconvoluted components from the shaded area of the main profile. **A** isoleucine (2TMS), $\text{M/Z} = 158$; **B** threonine (2TMS), $\text{M/Z} = 117$; **C** proline (2TMS),

$M/Z = 142$; **D** glycine (3TMS), $M/Z = 174$; **E** 2,2,3,3-d₄-succinic acid (2TMS), $M/Z = 251$; **F** succinic acid (2TMS); $M/Z = 247$ (factor of magnification 10). The presence of 2,2,3,3-d₄-succinic acid resulted from standard addition of a deuterated isotopomer.

Figure 4 depicts a clustering tree of identified, and non-identified MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741 and pure standard compounds. MSTs were classified into groups by hierarchical clustering of a complete symmetric matrix of pair-wise mass spectral match values (Table 4). 18 groups of MSTs were classified at a cut-off at approximately 50 % diversity (the MST groups are described in Example 6).

Figure 5 shows the results of a principal component analyses based on GC-TOF-MS metabolite profiles of extracts from a single batch culture of *Saccharomyces cerevisiae* strain BY4741 ($A_{595} \sim 1.8$). Four sampling strategies ($n = 16$) were employed, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). Washes were performed with glucose-free SD medium. Principal components 1, 2, and 3 covered 57.4 %, 24.2 %, and 6.4 % of the total variance of the profile data set. Metabolite responses were normalised to the average metabolite response observed within each sample. Average relative standard deviation (RSD) of each of the sampling procedures is indicated. Underlying metabolite profiles, metabolite responses and relative standard deviations of all metabolites are presented in Table 6.

Figure 6 provides the results of a comparison of four co-response measures applied to metabolite profiles of *Saccharomyces cerevisiae* strain BY4741 ($A_{595} \sim 1.8$). Kendall's correlation coefficient is compared to Euclidian distance (A), mutual information (B) and Pearson's correlation coefficient (C). Each tuple represents a metabolite/metabolite co-

response. Arrows indicate position of exemplary bi-plots presented in double-log₁₀ scale to the right. Four sampling strategies (n = 16) were employed, namely MEOH, FILTER, SPIN, and SPINW. The sampling techniques were as described within the legend to Figure 5. A complete overview of all pair-wise metabolite/metabolite co-response measures is given in Table 7.

Figure 7 shows metabolite bi-plots in double-log₁₀ scale representing co-response behaviour of intermediates and a product of the tricarboxylic acid cycle. Oxaloacetic acid was below limits of detection in GC-TOF-MS profiles of yeast. **A**, malic acid/ aspartic acid; **B**, malic acid/ citric acid; **C**, fumaric acid/ malic acid; **D**, succinic acid/ fumaric acid. The sampling techniques are as described within the legend to Figure 5.

Figure 8 shows the common nearest and most distant neighbours of succinic acid, fumaric acid, and malic acid, as described by Kendall's correlation coefficient. Values of correlation coefficients were coded by line style, ≥ 0.6 full line and ≤ -0.5 dotted line.

Figure 9 shows a continuous positive-ion MALDI-TOF-MS spectrum of an ambient $\delta^{13}\text{C}$ -yeast extract with 2,5-dihydroxybenzoic acid as matrix set to the expected mass range of NAD^+ (NADH) adducts, namely protonated molecular ions at m/z 664.11 (666.13), and sodium adducts at m/z 686.09 (688.12), respectively. The inset ($^{12}\text{C}/^{13}\text{C}$) shows a bar representation of the protonated molecular ion region from a ^{13}C -isotopomer ratio (^{13}C -ITR) MALDI-TOF-MS analyses. m/z 679.26 and 681.25 represent protonated NAD^+ and NADH , which were labeled with 15 ^{13}C -atoms. ^{13}C -saturated yeast extracts exclusively showed the labeled ions in the m/z 677 - 685 range (data not shown).

Figure 10 depicts a head-to-tail analyses of post source decay (PSD) fingerprints from separate MALDI-TOF-MS analyses of ambient $\delta^{13}\text{C}$ - (^{12}C PSD) and ^{13}C -saturated (^{13}C PSD) yeast extracts. Evident m/z differences of

parent ions and fragments were 15, 10, and 5 amu. The required mass window for the isolation of parent ions ($\sim \pm 3$ amu) and subsequent PSD analyses did not allow separate monitoring of NAD^+ and NADH from mixtures.

The following Examples illustrate the invention:

Experimental set-up

Strain information and in-vivo labeling

Saccharomyces cerevisiae strains BY4741 (MATa; his3 Δ 1; leu2 Δ 0; met15 Δ 0; ura3 Δ 0) and BY4742 (MAT α ; his3 Δ 1; leu2 Δ 0; lys2 Δ 0; ura3 Δ 0) were obtained from the EUROFAN II worldwide gene deletion project (EUROSCARF collection, Frankfurt, Germany. http://www.uni-frankfurt.de/fb15/mikro/euroscarf/col_index.html) (Kelly, 2001; Winzeler, 1999). Strains were grown for 16-24 h in 25 - 250 ml liquid batch cultures on synthetic defined (SD) minimal medium with required auxotrophic supplementation and 20 g l⁻¹ ambient $\delta^{13}\text{C}$ -glucose as major carbon source (Castrillo, 2003). For in-vivo ^{13}C -labeling ambient glucose was replaced by U- ^{13}C -glucose (99 atom %, Isotech Inc., Miamisburg, USA). Auxotrophic and vitamin supplements were non-labeled.

For the control of residual SD medium components within cellular preparations from yeast cultures the media contained 4 g l⁻¹ lactose (β -D-galactopyranosyl-(1,4)-D-glucose, Fluka, Buchs, Switzerland), which is not utilized by *Saccharomyces cerevisiae*.

Cellular preparations from yeast cultures

For all experiments 5 ml aliquots were taken from over-night yeast batch cultures grown to $A_{595} \sim 1.8$. Sampling procedures were: (1) MEOH, quenching into -50°C cold methanol, subsequent centrifugation, and aspiration of supernatant (MEOH) (Castrillo, 2003; Gonzalez, 1997) with non-buffered quenching solution (see below);

(2) FILTER, vacuum collection onto 0.65 μm Durapore PVDF hydrophilic membrane filter discs (Millipore GmbH, Schwalbach, Germany); (3) SPIN, collection by gentle centrifugation and complete aspiration of supernatant without subsequent wash; (4) SPINW, collection by 2 repeated gentle centrifugation and wash cycles with carbohydrate-free SD media. All procedures were performed at 28°C if not mentioned otherwise. Cellular preparations were either immediately processed or shock frozen in liquid nitrogen. Routine sampling was MEOH, if not indicated otherwise. As monitored by the lactose-tracer molecule all sampling methods except SPINW contained low amounts of residual media components. Non-sample control experiments with fresh SD media and analyses of the initial cell free medium and at time of sampling were performed (data not shown).

Preparation of intracellular yeast metabolites

Hot methanol/ chloroform extraction (15 min at 70°C), liquid phase partitioning into methanol/water (1:1, v/v), drying by vacuum centrifugation, and subsequent treatment with methoxyamine hydrochloride (MEOX) and N-methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA) reagents for conventional yeast metabolite profiling of polar soluble material was down-scaled as described previously (Wagner, 2003). For the extended GC-TOF-MS analyses of yeast samples liquid partitioning by addition of water to the initial methanol/ chloroform extract was omitted. Instead the complete extract volume, ~ 700 μl , was dried by vacuum centrifugation.

Supplementation of quenching- or extraction-solution with recommended buffer systems (Castrillo, 2003; Gonzalez, 1997) for the preparation of intracellular yeast metabolites led to strong interferences of the buffer substances with either methoxyamination, silylation, or chromatographic performance of the final sample preparations. Therefore, buffering substances had to be avoided for GC-MS profiling.

^{13}C -isotopomer ratio (ITR) metabolite profiling

Extracts of intracellular yeast metabolites from ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated cultures were combined in equal amounts prior to vacuum centrifugation. The ^{13}C -

saturated extract was treated as a stable isotope labeled, multiplex internal standard mixture. Each component of the resulting metabolite profiles was quantified by use of the respective ^{13}C -saturated compound. For this purpose $^{12}\text{C}/^{13}\text{C}$ response ratios of pre-selected isotopomer fragment pairs were calculated (Table 2). Specific isotopomer fragment pairs were assigned manually to each identified and non-identified metabolite using respective mass spectral entries from the collection of mass spectral metabolite tags (MSTs; see below). Prior to forming ratios responses of ^{13}C -saturated fragments were corrected for the contribution of naturally occurring ^{13}C -isotopomers to ambient $\delta^{13}\text{C}$ -preparations.

GC-MS technologies

Conventional GC-MS profiles were performed with a quadrupole type GC-MS system, namely a GC8000 gas chromatograph coupled to a Voyager mass spectrometer, which was operated by MassLab software (ThermoQuest, Manchester, UK). Modifications to the initial GC-MS profiling method (Fiehn, 2000a; Fiehn, 2000b) were, injection of 1 μl sample in splitless mode, use of a 5°C min^{-1} temperature ramp with final temperature set to 350°C on a 30 m x 0.25 mm inner diameter Rtx-5Sil MS capillary column with an integrated guard column (Restek GmbH, Bad Homburg, Germany), and use of alkane mixtures for the determination of retention time indices. These changes reflect recent optimisation which was performed with a GC-TOF-Pegasus II MS system (Leco, St. Joseph, USA). All GC-TOF-MS experiments were done on a Pegasus II TOF-MS system as detailed earlier for a diverse range of plant samples (Wagner, 2003)

MALDI-TOF-MS technologies

Yeast extracts were analysed by MALDI-TOF-MS (Voyager DE-PRO Biospectrometry Workstation, Applied Biosystems, Foster City, USA) set to positive ion detection in reflectron mode (Lerouxel, 2002). Settings for reflectron MALDI-TOF-MS and PSD were as recommended by the manufacturer. A 2,5-dihydroxybenzoic acid (10 mg ml^{-1}) matrix was mixed 1:1 (v/v) with polar fractions from yeast extracts

or pure compounds, which were dissolved in methanol: water (1:1, v/v). Slow crystallisation by air drying was essential for the laser desorption and ionisation of NAD⁺ and NADH; microcrystalline samples exhibited complete signal suppression. An exemplary study using the same MALDI-TOF-MS matrix previously demonstrated that stable isotope standardized MALDI-TOF-MS exhibited precise standard curves over two orders of magnitude and produced quantitative results in accordance with in-parallel gas chromatographic analyses (Kang, 2001).

Generation of a compendium MST library

MSTs (Table 3) were obtained through automated deconvolution of GC-TOF-MS chromatograms (ChromaTOF™ software, LECO, St. Joseph, USA). Mass spectra were collected into user libraries provided by NIST98 and AMDIS software (http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html and <http://chemdata.nist.gov/mass-spc/amdis/>; National Institute of Standards and Technology, Gaithersburg, USA) (Stein, 1999; Ausloos, 1999). MSTs were manually annotated and corrected for obvious errors caused by automated deconvolution. Mass spectra of low intensity and truncated or fused mass spectra which resulted from co-elution of compounds were rejected except for demonstrating of the presence of a labeled isotopomer.

Identification and classification of mass spectral metabolite tags (MSTs)

MSTs were identified by manually supervised standard addition experiments with pure commercially available substances. Required criteria for substance identification were chromatographic co-elution and high mass spectral similarity of MSTs observed within yeast samples to standard substances (Wagner, 2003). Co-elution and similarity were described by retention time index and mass spectral match values, respectively. Non-identified MSTs were tentatively analysed by best match with a customised MS library of standard substances and entries from the commercial NIST98 library (National Institute of Standards and Technology, Gaithersburg, USA). MSTs were classified by agglomerative hierarchical cluster analyses using Euclidian

distance measure and average linkage (Table 5, Figure 4). Cluster analyses was applied to a complete matrix of pair-wise mass spectral match values (Table 4) as described earlier (Wagner, 2003). Yeast MSTs and a selection of EI-TOF mass spectra from pure standard substances were co-classified.

Statistical analyses and visualisation of metabolite profiles

Principal component analyses (PCA), hierarchical clustering, calculation of Euclidian distance, Pearson's and Kendall's correlation coefficient, and mutual information was calculated using the S-Plus 2000 software package standard edition release 3 (Insightful, Berlin Germany), the programming language R version 1.6.1 and 1.6.2 (<http://www.r-project.org>) and the MetaGeneAlyse version 1.3 world wide web resource (<http://metagenealyse.mpimp-golm.mpg.de/>) (Daub, 2003).

The model for metabolic network representation was as suggested (Jeong, 2000) and overlay of correlation coefficients in accordance with modularity analyses in metabolic networks (Ravasz, 2002). Network visualisation and layout was performed using the Pajek (Batagelj, 1998) algorithm package available at <http://vlado.fmf.uni-lj.si/pub/networks/pajek/>.

Calculation of metabolite profiles

Each metabolite was represented by a single response value (Table 6). Within GC-MS profiles single metabolites may be represented by multiple derivatives, which are detected by respective MSTs, and each MSTs may be represented by more than one specific fragment (refer to Table 2 and Figure 1). In these cases an additive composite metabolite response was calculated rather than selecting a single MST and corresponding fragment.

Metabolite response was normalised to the average signal intensity of all MSTs, which were observed within each single GC-MS chromatogram. This strategy of data normalisation was mandatory prior to comparison of sampling technologies and analyses of metabolite co-response, because sampling technologies had variable and different recoveries of viable cells from the same batch culture. For example,

each wash cycle of SPINW sampling successively reduced recovery of viable cells (data not shown). Attempts failed to identify a constitutive metabolite, which would allow to exactly monitor the number and size of viable yeast cells within each preparation.

Example 1: Determination of the extent of saturation by in vivo ^{13}C -labeling

In order to determine the completeness of in vivo ^{13}C -labeling (saturation), yeast cells (yeast strain BY 4741; Kelly, 2001; Winzeler, 1999) were fed with U- ^{13}C -glucose as the only carbon source except for auxotrophic and vitamin supplements, i.e. biotin, pantothenate, folic acid, inositol, niacin, p-aminobenzoic acid, pyridoxine, riboflavin, thiamine, bacto-yeast nitrogen base without amino acids, histidine, leucine, methionine, uracil, and inorganic salts, i.e. ammonium sulfate, boric acid, copper sulfate, potassium iodide, ferric chloride, manganese sulfate, sodium molybdate, zinc sulfate, potassium phosphate, magnesium sulfate, sodium chloride, calcium chloride that were non-labeled and extracts from these yeast cells were examined by conventional electron impact GC-MS for the content of different metabolites. As judged by the resulting mass spectra profiles, the majority of the detectable metabolites from the yeast cells was completely labeled. In detail, ambient (i.e. naturally occurring) $^{12}\text{C}/^{13}\text{C}$ -carbon ($\delta^{13}\text{C}$ -) isotopomer composition was found for uracil, methionine, histidine, nicotinic acid and inositol in extracts prepared from cultures supplemented with U- ^{13}C glucose. Non-labeled leucine and pantothenic acid were frequently observed, however these metabolites were only abundant at levels close to detection limits. Other vitamins comprised by SD media, e.g. biotin, folic acid, p-aminobenzoic acid, pyridoxine, riboflavin, and thiamine, were below limits of detection or not accessible by GC-MS technology.

Furthermore, homocysteine, and inositol-phosphate were detected devoid of ^{13}C -label. A still non-identified conjugate of inositol exhibiting high similarity to galactinol was partially labeled, and uridine carried 5 out of 9 possible ^{13}C atoms. These findings indicate: (1) synthesis of homocysteine from methionine by 5-methyltetrahydropteroyltri-L-glutamate:L-homocysteine S-methyltransferase (EC 2.1.1.14; MET6), (2) a pathway from inositol to inositol-phosphate possibly through

phosphatidylinositol synthase (2.7.8.11; PIS) and phospholipase C (3.1.4.11; PLC1) activity, and (3) uracil scavenged by uracil phosphoribosyltransferase (EC 2.4.2.9; FUR1) and subsequent phosphatase action.

Example 2: "Inverse labeling" of yeast cells

L-lysine supplementation of yeast strain BY 4741 was tested in ^{13}C -saturated cultures. Lysine is the complementary auxotrophic marker substance of the second *Saccharomyces cerevisiae* strain BY4742 used by the EUROFAN II worldwide gene deletion project (Kelly, 2001; Winzeler, 1999). ^{13}C -labeling of lysine was suppressed in strain BY4741 when supplemented with this amino acid. Moreover, 2-aminoadipic acid accumulated only in strain BY4742. This results indicates that the bi-directional L-lysine synthesis and degradation pathway which comprises the activities of L-aminoadipate-semialdehyde dehydrogenase (EC 1.2.1.31; LYS2, LYS5), NADP^+ , L-glutamate-forming saccharopine dehydrogenase (EC 1.5.1.10; LYS9), and NAD^+ , L-lysine-forming saccharopine dehydrogenase (EC 1.5.1.7; LYS1) is interrupted.

Example 3: Identification of ^{12}C - and ^{13}C -isotopomer pairs

Reliable identification of pairs of ^{12}C - and ^{13}C -isotopomers which represent the same metabolite is a prerequisite for accurate isotopomers ratio (ITR) metabolite profiles. Pairs of isotopomers may be identified based on mass spectral fragmentation as well as by chromatographic retention. Initial GC-MS experiments demonstrated that derivatives of commercially available deuterated compounds had significantly smaller retention time indices (RI) than non-deuterated compounds. For example, 2,3,3,3-D₄ alanine (2 TMS), 2,3,3-D₃-aspartic acid (3 TMS), 2,3,3,3-D₄ alanine (3 TMS), 2,2,3,3-D₄-succinic acid (2 TMS), and 2,3,4,4,4,5,5,5-D₈- valine (2 TMS) eluted 1.1, 1.8, 2.3, 2.5, and 3.8 RI units prior to respective non-deuterated isotopomers.

In contrast, commercially available ^{13}C -labeled compounds exhibited only minor shifts in RI. This observation was confirmed by a selection of 66 ^{13}C -labeled mass spectral metabolite tags (MSTs) observed in standard GC-MS profiles. This testing set of MSTs was selected according to high mass spectral peak purity and presence

of at least one abundant and specific fragment which could be employed for selective ion quantification and RI monitoring. The selection comprised derivatives of amino acids, organic acids, sugars, sugar alcohols, sugar phosphates, and a set of 34 non-identified MSTs. The complete list including all available and manually evaluated GC-EI-MS isotopomer fragment pairs is listed in Table 2 (see *infra*). RI of ^{13}C -labeled compounds was on average only $0.28 (\pm 0.53 \text{ SD})$ units smaller than those of non-labeled compounds. This slight shift of RI was equivalent to approximately 0.3 sec of retention time.

Interpretation of the EI-MS fragmentation pattern of pairs of ambient $\delta^{13}\text{C}$ - and ^{13}C -isotopomers allowed the verification of metabolite identity. Typical EI mass spectra of succinic acid (2 TMS), glycine (3 TMS), and glutamic acid (3TMS), are shown in Figure 1. The head to tail analyses of ambient $\delta^{13}\text{C}$ - and ^{13}C -EI-mass spectra allowed an easy identification of isotopomer fragment pairs for use in ITR metabolic profiling. For example, glutamic acid ($\text{C}_5\text{H}_9\text{NO}_4$) forms a TMS derivative with the sum formula $\text{C}_{14}\text{H}_{33}\text{NO}_4\text{Si}_3$ and a relative molecular mass of 363. The molecular ion M^+ , m/z 363, and the $[\text{M}-15]^+$ fragment, m/z 348, which is generated by typical neutral loss of a CH_3 -radical from a TMS group, correspond to ions being characterized by m/z 368 and m/z 353 in which all 5 carbon atoms of glutamic acid are ^{13}C -labeled. The fragment $[\text{M}-117]^+$, m/z 246, can be matched with the corresponding ^{13}C -isotopomer fragment, m/z 250. These fragments are formed by neutral loss of a trimethylsilylated carboxyl group, which contains one of the 5 carbon atoms of the glutamic acid. The M^+ and $[\text{M}-15]^+$ fragments of ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated succinic acid (2 TMS), glycine (3 TMS) and glutamic acid (3TMS) are shown in the insets of Figure 1. These mixed mass spectra were obtained from ^{13}C -ITR metabolite profiles, i.e. combined analyses of ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast extracts within single chromatograms. The chosen examples also demonstrate the necessity to correct ^{13}C -ITR metabolite profiles for ambient ^{13}C -isotopomer abundance, especially when the available mass spectral fragments for ^{13}C -ITR metabolite profiles contain only 1 or 2 labeled carbon atoms.

Example 4: Comparison of ^{13}C -ITR metabolite profiles with conventionally produced metabolite profiles

^{13}C -ITR metabolite profiles produced by combining equal amounts of ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast extracts into one GC-MS analyses were compared with conventional, i.e. separate, GC-MS profiles of the same extracts. The above-mentioned testing set of yeast MSTs was used for this comparison. Each MST was quantified by up to 3 manually validated isotopomer fragment pairs Table 2 (see *infra*). This experiment was performed with the aim to establish whether ITR metabolite profiling which utilizes internal standardisation by each the ^{13}C -labeled compounds is equivalent with conventional metabolite profiling. The latter approach was shown previously to operate successfully by external quantification (Fiehn, 2000a; Roessner, 2000).

Two yeast cultures were grown from the same colony in liquid SD medium. One culture was supplemented with ambient $\delta^{13}\text{C}$ -glucose, the second with U- ^{13}C -glucose. Extracts of these cultures were either analysed separately or combined for ^{13}C -ITR before derivatisation. An initial experiment (Exp1) was repeated by taking a second sample from the same culture after a 15 min time interval (Exp2).

Two comparisons were performed based on the resulting metabolite profiles. (1) Comparison of Exp1 with Exp2 demonstrated the analytical variability, by means of re-analysing the same cultures (Figures 2C and 2D). (2) Comparison of the GC-MS responses of the labeled and non-labeled isotopomer fragment pairs showed the effect of ^{13}C -saturation on metabolic profiles (Figures 2A and 2B). Both comparisons were done either by ITR metabolite profiling (Figures 2A and 2C; ITR GC-MS analyses 06 and 10) or by conventional metabolite profiling (Figures 2B and 2D; ambient $\delta^{13}\text{C}$ GC-MS analyses 04 and 08; ^{13}C -saturated GC-MS analyses 05 and 09). GC-MS analyses 04, 05 and 06 represented Exp1, while analyses 08, 09, and 10 comprised Exp2. Pearson's linear correlation coefficient applied to the comparison of the experiments as well as to the influence of ^{13}C -saturation on the metabolic profiles demonstrated equivalence of ITR metabolite profiling and conventional metabolite profiling (Figure 2, inset).

The average coefficient of variation was determined by using all fragment pairs which contributed to each of the comparisons. Again results of ITR metabolite profiling and conventional metabolite profiling were equivalent, however, average coefficients of correlation were smaller in ITR metabolite profiling analyses (Figure 2, inset).

Most of the labeled isotopomers from the ^{13}C -saturated culture were present in amounts almost equal to the ^{12}C -isotopomers from the ambient $\delta^{13}\text{C}$ -culture. The average $^{12}\text{C}/^{13}\text{C}$ -isotopomer ratio of all pairs from the complete MST testing set was 0.79 (± 0.40 SD). However, some substances exhibited extreme differences, the ratios ranging between 0.01 and 2.98. These observations indicated that the process of ^{13}C -saturation alone may alter the levels of metabolites. Therefore, ITR metabolite profiling analyses of multiple samples should be standardised by extracts from a single large ^{13}C -saturated culture and corrected for the systematic error of ^{13}C -labeling.

Example 5: Preparation of a compendium of MSTs

Compilations of MSTs from biological samples represent an approach analogous to sequencing projects of expressed sequence tags (EST). We characterised the relevant major metabolites of yeast samples, obtained mass spectra and retention time indices for reliable metabolite identification, and finally generated means for metabolite-specific relative quantification.

Recently introduced GC-TOF-MS technology (van Deursen, 2000; Wagner, 2003) was adapted to the metabolic profiling of yeast. Fast scanning GC-TOF-MS systems are ideally suited for metabolite compendium projects. These systems allow automated and comprehensive deconvolution of mass spectral components from highly complex samples without user intervention. Moreover, this novel technology combines the advantages of high chromatographic resolution and reproducibility with the equally high reproducibility and acquisition rate of non-scanning time-of-flight MS-technology. In vivo stable isotope labeling was used to facilitate one of the most time-consuming steps in establishing metabolite profiling of any given biological sample type, i.e. the task to differentiate between MSTs which originate from yeast metabolism and MSTs which represent experimental contaminations. The stable isotope label was introduced as a chemically defined and predominant carbon source and was used to detect all metabolic conversions originating from this carbon source. The apparent complexity of initial metabolic profiles of polar extracts from yeast was lower than profiles generated for instance from plant sources. We increased the final

efficiency of multi-parallel GC-TOF-MS analyses by adapting metabolic profiling to combined chloroform and methanol extracts from yeast which contained lipid metabolites in addition to the metabolites obtained by polar extraction as described earlier. Further attempts to increase the amount of yeast extract to be applied to GC-TOF-MS analyses in order to maximise the number of simultaneously monitored compounds were limited by matrix effects, which were brought about by four predominant compounds, phosphoric acid (3TMS), glycerol (3TMS), glucose (MX, 5TMS), and trehalose (8TMS). The matrix effects resulted (1) from excess phosphoric acid within extracts, which reduced the silylation strength of the MSTFA reagent and (2) from chromatographic overload of derivatives which produced peak deformation artefacts in the vicinity of major peaks. The final amount of yeast extract was adjusted to avoid these matrix effects (Figure 3). Thus the efficiency of multi-parallel GC-TOF-MS analyses was increased, for the time being without introducing time-consuming pre-fractionation and enrichment protocols.

A compendium of GC-TOF-MS metabolite tags was separately compiled from ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated yeast extracts from over-night batch cultures of *Saccharomyces cerevisiae* strain BY4741. In order to obtain different samples the metabolite profiles of which can be compared, different sampling protocols were applied, namely quenching into cold methanol (MEOH), collection onto filter disc (FILTER), collection by centrifugation without media wash (SPIN), and collection by repeated wash and centrifugation cycles (SPINW). The initial set of automatically retrieved mass spectra was manually curated to select MSTs of metabolic origin. The criteria applied for curation were: repeated occurrence of the mass spectral component ($n > 3$), reproducible fragment composition, signal to noise ≥ 50 , and presence of a co-eluting ^{13}C -isotopomer. Mass spectra of metabolite derivatives devoid of carbon, and metabolite derivatives originating from ambient $\delta^{13}\text{C}$ auxotrophic and vitamin supplementation were included. The MST compendium is depicted in Table 3.

Example 6: Identification and classification of MSTs

For the identification of MSTs, mass spectral matching algorithms were employed, which are contained in publicly available mass spectral search and comparison software (Stein, 1999; Ausloos, 1999). The underlying procedures are analogous to those employed in BLAST analyses of ESTs. MSTs were compared to commercial MS collections and a custom EI-TOF-MS library. Best matches were assigned for a preliminary identification (Table 3). However, the presence of multiple chemical isomers with close to identical mass spectral fragmentation patterns make it necessary to conduct standard addition experiments in order to obtain a precise identification. We sampled 180 MSTs (Table 3) and identified 78 tags which represented 67 yeast metabolites (Table 1). The range of identified compounds comprised amino acids, organic acids, sugars, polyols, purines and pyrimidines, phosphorylated compounds, fatty acids and sterols (Table 1).

A non-biased, automated classification of MSTs has previously been established (Wagner, 2003). This approach towards a non-biased mass spectral classification utilises the observation that two mass spectra of the same compound do not only match best but also have similar match values when compared to other, even highly different, mass spectra. This method of MST classification was applied to yeast MSTs and a framework of known mass spectra obtained from standard addition experiments. We inferred 19 groups of MSTs from agglomerative hierarchical clustering by average linkage of Euclidian distances and a cut-off at approximately 50 % diversity (Figure 4 and Table 5). The groups of MSTs comprised alkanes which were included for RI standardisation (group 1; 0/7 non-identified), di- and tri saccharides (group 2; 4/17 non-identified), hexose pyranosides (group 3; 8/9 non-identified), hexonic acids and inositol (group 4; 4/10 non-identified), aldohexose methoxyamines (group 5; 3/12 non-identified), a group of non-identified MSTs similar to polyols (group 6; 5/5 non-identified), ketohexose- and pentose methoxyamines (group 7; 0/14 non-identified), hexitols, pentitols and hexonolactones (group 8; 2/19 non-identified), a group of standard caffeoylquinic acids (group 9; 0/8 non-identified), organic acids and purine nucleosides (group 10; 8/34 non-identified), C3-C5 polyols, hydroxy acids and sugars (group 11; 9/30 non-identified), phosphates (group 12; 9/34 non-identified), amines and amino acids with primary amino-group (group 14; 8/26 non-identified), fatty acids and sterols (group 15; 7/15 non-identified), a standard set of phenylpropanoic acids (group 16; 0/9 non-identified), a heterogenous group of

mostly cyclic compounds comprising phenyl-, indoyl-, imidazol-, pyrimidine-, and purine-residues (group 17; 12/31 non-identified), and a group dominated by amino acids (group 18; 9/60 non-identified). Group 0 (17 MSTs) and group 3 (4 MSTs) represented mass spectra with unclear classification. Most of those mass spectra, which represented identical compounds were found to be either nearest neighbours or were classified to belong to the same branches of the clustering tree. The mass spectrum of leucine (2TMS) was entered in duplicate in order to monitor the position of a pair of identical mass spectra within the clustering tree (Figure 4). Some yeast MSTs of group 0, namely methionine (2TMS), adenine (2TMS), and proline (2TMS), did not sort as expected. This observation was caused by errors of automated deconvolution due to low abundance or due to co-elution of other MSTs. Clustering after substitution of the matrix by a minimum threshold match value allowed improved grouping of missorted mass spectra, but obscured classification of those MSTs without high similarity to other MSTs or standard MS. More elaborate, preferably supervised-learning algorithms applied to matrices of match values as well as directly to mass spectra and RI will lead to improved and more precise classification results and increased robustness of identification.

Example 7: Application of metabolite profiling analyses

Metabolites are embedded within a network of fast enzyme and transport reactions. Not unexpectedly, metabolite co-response was discovered within sets of GC-MS metabolite profiles from plant samples. This co-response was subsequently discussed to yield novel information about biochemical mechanisms of metabolite interactions. Because reaction rates of metabolic conversions are in general significantly higher than rates of protein or mRNA turn-over, this type of analyses highly depends on a quick quenching of the metabolism during sample preparation. However, shock-freezing in liquid nitrogen, which was described earlier to be successful for plant samples, cannot be applied to yeast liquid cultures. For this reason, four other sampling regimes were assessed. These were applied to aliquots from a single batch culture. The sampling strategies were as described above (see Example 5), namely MEOH-, FILTER-, SPIN-, and SPINW-sampling by two repeated wash and centrifugation cycles of SD medium without carbohydrate source. The

metabolic perturbation induced by the respective sampling technologies was monitored by GC-TOF-MS metabolite profiles.

Principal component analyses (PCA) of all GC-TOF-MS metabolite profiles demonstrated that each of the sampling strategies exhibited specific metabolic characteristics (Figure 5). Sampling by repeated wash and centrifugation cycles (SPINW) with glucose-free SD medium was distinct from SPIN sampling and other sampling methods as described by principal component 1, which comprised the bulk variance, 57.4 %, of this experiment. Component 2, which held 24.2 % of total variance, separated sampling by centrifugation, i.e. SPIN and SPINW, from other sampling technologies. Component 3 comprising 6.4 % of total variance still allowed separation of MEOH from FILTER samples. All subsequent principal components were of low descriptive value with respect to the effect of the four sampling technologies. Analyses of the first three component loadings showed that lysine, asparagine, leucine, homoserine, methionine, arabinose, glycerol, octadecanoic acid, and 15 non-identified MSTs contributed most to the variance introduced by the choice of experimental perturbation (Table 6).

All sampling methods tested had a similar range of reproducibility as was indicated by the average relative standard deviation (RSD) of all replicate metabolite measurements (Figure 5). However, reproducibility of metabolite measurements were in some cases much lower than observed in plant samples. For example, the most widely accepted method, i.e. sampling of yeast cultures into cold methanol (MEOH), exhibited high variation for aspartic and glutamic acid, 67.2 % and 91.6 % RSD, respectively. This high variance was not caused by a trend over time of sampling or GC-TOF-MS analyses. In contrast, we demonstrated that other sampling strategies allowed highly reproducible measurements of these compounds, as was indicated for example by 18.0 % RSD with aspartic acid after FILTER sampling and 7.0 % RSD with glutamic acid after SPINW sampling. A complete overview of detailed metabolite-specific data is given in Table 6.

The data provided herein point toward the conclusion that some metabolite pools were in fast transition during or in between MEOH sampling. With respect to some metabolites, for example aspartic acid (Figure 7A) and glutamic acid, fast SPIN sampling was highly similar to MEOH sampling in exhibiting rapidly changing

metabolite pools. Finally, slower sampling technologies, like FILTER and SPINW, apparently allowed adjustment of stable metabolite pools prior to sampling.

Example 8: Metabolite co-response analyses

The analyses presented in Example 7 appear to reflect rapidly changing pool sizes of some metabolites. Thus, the metabolic perturbations, which were caused by the sampling procedures, were employed in order to gain insight into metabolite/metabolite interactions. Four co-response measures, namely Pearson's correlation coefficient, Kendall's correlation coefficient, mutual information (Steuer, 2002), and Euclidian distance, were applied to characterise all pair wise metabolite combinations. The results of these analyses are shown in Table 7.

Pearson's correlation coefficient and Kendall's correlation coefficient were applied to screen for linear co-response, which was reported to prevail in similar analyses of plants. The combination of both parametric and non-parametric tests allowed a preliminary evaluation of the import of outlying measurements on each metabolite co-response. Only a small fraction of apparent linear metabolite co-responses were caused by outlying metabolite measurements (Figure 6C). When comparing Kendall's and Pearson's correlation coefficients, which were applied to the same metabolite pairs, we observed a roughly sigmoidal relationship with positive and negative linear correlation distributed almost equally. A typical example of a negative linear co-response referring to the metabolite pair glycine/uracil is shown in Figure 6C.

Mutual information of metabolite pairs plotted over Kendall's correlation coefficient shows a minimum at Kendall's correlation coefficient close to zero. The mutual information measure confirmed positive and negative linear co-response. Moreover, selecting metabolite pairs with high mutual information and low Kendall's correlation coefficient allowed to discriminate non-linear or, as shown for glycine and alanine (Figure 6B), conditionally linear metabolite co-response.

Euclidian distance proved to be a measure apparently independent of linear correlation (Figure 6A) or mutual information (data not shown). Euclidian distance, however, was highly efficient in selecting metabolite co-responses which exhibited low variance of both metabolites.

Because each of the correlation measures had different properties, it was refrained in the present work from global hypothesis-free metabolite classification through cluster analyses based on any single distance measure. Instead by selecting intermediates and products of the tricarboxylic acid cycle, we posed the question as to whether the metabolites of a common pathway may be correlated. Succinic acid, fumaric acid, malic acid, aspartic acid, and citric acid were covered by the GC-TOF-MS analyses of yeast cultures presented herein. Aconitic acid, isocitric acid, and 2-oxoglutaric acid can be analysed by GC-TOF-MS profiling but were below limits of detection in this experiment. In a first approach, we focused on those metabolite co-responses which refer to direct links by biochemical reactions (Figure 7). Highly linear correlations were observed for succinic acid, fumaric acid and malic acid, which were maintained throughout all types of sampling (Figures 7C and 7D). By contrast, malic acid and citric acid or aspartic acid, respectively, adopted seemingly independent sampling specific states (Figures 7A and 7B). These states were either linear (Figures 7A and 7B; FILTER subset) or of highly variable and non-linear nature. Other metabolites, which are known to be directly interlinked by biochemical reactions, were also found to be correlated, for example lanosta-8,24-dien-3-beta-ol and ergosterol, glucose-6-phosphate and fructose-6-phosphate, or hexadecanoic acid and octadecanoic acid (Table 7).

In addition, interactions which did not follow classical pathway definitions were found within the data set of metabolite co-responses. For example, we selected a group of corresponding metabolites from a biochemical path of interest, namely succinic acid, fumaric acid, and malic acid, and searched for common closest neighbours. The 3 closest neighbours of this group of organic acids were glyceric acid and two non-identified metabolites as judged by positive Kendall's correlation coefficient. In addition lysine, glycine, and glutamic acid were most distant as judged by negative Kendall's correlation coefficient. An overview of this analyses is shown as a network representation (Figure 8).

Example 9: ¹³C-ITR metabolite profiling by MALDI-TOF mass spectrometry

Metabolite profiling by GC-TOF-MS was shown to cover about 11% of the 584 yeast metabolites which were predicted by genome-scale reconstruction (Forster, 2003). However, this approach is mainly restricted by the limited scope of the GC-TOF-MS technology. The focus on specific classes of compounds with common properties is inherent to this as well as to any other analytical technology. For this reason, it is demonstrated in connection with the present invention that metabolite profiling using ^{13}C -in vivo labeling can be extended to MALDI-TOF-MS. MALDI-TOF-MS represents a mass spectral technology, which (1) cannot rely on chromatography for the confirmation of substance identity, (2) is highly sensitive to matrix suppression effects during laser desorption and ionisation, and (3) is not suited for external quantitative calibration. However, using MALDI-TOF for quantification with internal standard substances which are labeled by stable isotopes is an accepted procedure in connection with metabolite flux analyses (Wittmann, 2002; Wittmann, 2001). By nicotinamide adenine dinucleotide (NADH; $\text{C}_{21}\text{H}_{29}\text{N}_7\text{O}_{14}\text{P}_2$), an ubiquitous metabolic co-factor was chosen which allowed the demonstration of prerequisites essential to the ^{13}C -ITR approach.

Yeast extracts were treated as described above (see Example 4) to yield samples of a third experiment (Exp3). These samples were each harvested from the same batch cultures. Extracts with ambient $\delta^{13}\text{C}$ composition, extracts with ^{13}C -saturated metabolites, and an equal mixture of both extracts were analysed. Screening of MALDI-TOF spectra from the ambient $\delta^{13}\text{C}$ extract revealed protonated molecular ions of NAD^+ and NADH at m/z 664.11 and m/z 666.13, as well as sodium adducts at m/z 686.09 and 688.12 (Figure 9). These identifications were supported by commercial preparations of NAD^+ and NADH. The mass resolution of the MALDI-TOF system did not allow separation of the mono-isotopic ^{12}C -NADH ion from the A+2 isotopomer of ambient NAD^+ . Therefore, analogous to the quantification of glycine (3TMS) (Figure 1), correction will be required for the determination of NADH in the presence of NAD^+ . In addition, MALDI-TOF generated a continuous evenly spaced background of signals (Figure 9).

Within the mixed sample (Figure 9, inset), we found isotopomers of the protonated molecular ions of NAD^+ and NADH, which contained 15 ^{13}C -atoms out of 21 carbon atoms present within NAD(H). Small amounts of labeled sodium adducts were present (data not shown). The presence of only 15 labeled carbon atoms was in

agreement with the incorporation of non-labeled nicotinamide moieties into NAD(H), which originated from the nicotinic acid vitamin supplement contained in the yeast SD medium. The presence of non-labeled nicotinic acid ($C_6H_5NO_2$) in ^{13}C -labeled yeast extracts was demonstrated above (Example 1).

The identification of NAD(H) within yeast extracts was confirmed by post source decay (PSD) fingerprints of the protonated molecular ion cluster which were recorded separately from the ambient $\delta^{13}C$ and the ^{13}C -saturated yeast extracts (Figure 10). Analogous to the comparison of GC-EI-MS fragmentation pattern of isotopomers (Figure 1), head-to-tail analyses of PSD fingerprints allows the verification of the correct choice of isotopomer pairs. Moreover, fragment analyses of the ^{12}C -PSD and the ^{13}C -PSD revealed the successive loss of three moieties containing 5 carbon atoms each, namely two ribose units and one adenine building block, as was indicated by mass differences of 5, 10, and 15, respectively. Due to the restricted resolution of PSD analyses, separate fingerprints of the protonated ions of NAD^+ and NADH could not be obtained from mixtures. However, commercially available preparations of NAD^+ and NADH indicated that some PSD fragments, for example the fragment m/z 649.4 $[M-17]^+$, were highly specific. Fragment m/z 649.4 may result from facilitated neutral loss of NH_3 from the protonated NADH molecular ion. MALDI-TOF preparations of commercially available NAD^+ exhibited variable amounts of NADH mainly in the form of ion m/z 666.13, whereas NAD^+ was not detectable in preparations from NADH. This last finding indicated that the chosen MALDI-TOF procedure generates a reducing environment for chemical analyses which requires monitoring.

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Table 1

Table of yeast metabolites, which were represented by at least one mass spectral tag (MST). Identification of MSTs was performed by standard addition experiments. Identification required co-elution, mass spectral similarity, and presence of differentially labeled isotopomers.

Amino acids

2-Aminoadipic acid
 Alanine
 Arginine
 Asparagine
 Aspartic acid
 Cysteine
 Glutamic acid
 Glutamine
 Glycine
 Histidine
 Homocysteine
 Homoserine
 Isoleucine
 Leucine
 Lysine
 Methionine
 Ornithine
 Phenylalanine
 Proline
 Pyroglutamic acid
 Serine
 Threonine
 Tryptophan
 Tyrosine
 Valine

Organic acids

Citramalic acid
 Citric acid
 Erythronic acid
 Fumaric acid
 Gluconic acid
 Glyceric acid
 Malic acid
 Pantothenic acid
 Succinic acid

Miscellaneous

Adenine
 Ethanolamine
 Nicotinic acid
 Uracil
 Urea

Fatty acids

9-(Z)-Octadecenoic acid
 Hexadecanoic acid
 Octadecanoic acid
 Octadecenoic acid

Sterols

Ergosterol
 Lanosta-8,24-dien-3-beta-ol

Sugars

alpha-D-Methylglucopyranoside
 Arabinose
 Ribose
 Fructose
 Fucose
 Glucose
 Isomaltose
 Mannose
 Trehalose

Polyols

Erythritol
 Glycerol
 myo-Inositol
 Mannitol
 Ribitol
 Sorbitol

Phosphates

Fructose-6-phosphate
 Glucose-6-phosphate
 Galactose-6-phosphate
 Glyceric acid-3-phosphate
 Glycerol-2-phosphate
 Glycerol-3-phosphate
 Phosphoric acid

Table 2

The table includes all manually evaluated GC-EI-MS isotopomer fragment pairs of identified and non-identified metabolite derivatives used for ^{13}C -ITR metabolite profiling. The table comprises names of metabolite derivatives or of best matches, mass spectrum identifier (MS-ID) for cross-referencing with Table 3, mass to charge ratio (M/Z) characterising the fragment isotopomer pairs and deviation of retention time indices (ΔRI).

Table 3

Datafile in the format *.msp^a containing all curated GC-EI-TOF-MS mass spectra of MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741.

The spectrum name was designed to allow sorting according to isotopomer, retention time index, experiment, and name, for example 12C_1625.9_1274EC17_Glutamic acid (3TMS) or 12C_1802.0_1313EC75_[706; Xylitol (5TMS)]. Retention time indices are as observed within the indicated experiment. Names represent identifications by co-elution and mass spectral match^b; names in brackets indicate non-identified compounds and include the best mass spectral match. The chemical ID field was used to group isotopomer mass spectra by a common mass spectral ID (MS-ID), for example 163001-10-1 and 163001-11-1 representing ambient $\delta^{13}\text{C}$ - and ^{13}C -saturated isotopomers of glutamic acid (3TMS). This identifier does not represent a CAS registry number. The formatting of this field is predefined by AMDIS software.

^a The file format *.msp can be imported into NIST98 and NIST02 mass spectral comparison software (to be downloaded from http://chemdata.nist.gov/mass-spc/Srch_v1.7/index.html or AMDIS software (to be downloaded from <http://chemdata.nist.gov/mass-spc/amdis/>).

^b By-products observed in preparations of reference substances were marked (BP).

Table 4

Matrix of all mass spectral similarities of the MSTs from yeast which are presented in Table 3. A complete pair-wise matching was performed with NIST98 mass spectral search and comparison software.

Table 5

Table of identified and non-identified MSTs from extracts of *Saccharomyces cerevisiae* strain BY4741 and pure standard compounds. MSTs were classified into groups by hierarchical clustering of the complete symmetric matrix of pair-wise mass spectral match values (Table 4). The resulting clustering tree is shown in Figure 4.

Table 6

Table of metabolite responses from GC-TOF-MS metabolite profiles of four sampling strategies ($n = 6$), namely MEOH-, FILTER-, SPIN- and SPINW-sampling by two repeated wash and centrifugation cycles. All samplings were performed on a single batch culture of *Saccharomyces cerevisiae* strain BY4741 ($A_{595} \sim 1.8$). Metabolite responses were normalised by the average metabolite response observed within each sample. MSTs and fragments which comprised the metabolite responses in this set of experiments are indicated. Metabolites exhibiting more than 75% missing data in all types of sampling strategies were removed. Table 6A depicts the raw data values which gave rise to the average values depicted in Table 6B.

Table 7

Table of all pair-wise metabolite/metabolite co-response measures. Number of available pair-wise measurements, Euclidian distance, mutual information, Kendall's- and Pearson's correlation coefficient were calculated from the metabolite responses presented in Table 6. The global information content of the correlation measures is demonstrated in Figure 6.

Table 2

DERIVATIVE [BEST MATCH; NAME]	MS-ID	ISOTOPOMER PAIR M/Z	Δ RI
Alanine (2TMS)	110001	116_118 190_192 218_221	0.00 0.00 0.18
Glycine (3TMS)	133001	174_175 248_249 276_278	0.00 0.00 0.36
Threonine (2TMS)	132001	117_119 219_221 130_133	0.57 0.93 -0.75
Alanine (3TMS)	138002	188_190 100_102 262_264	0.00 0.00 0.18
Serine (3TMS)	138001	204_206	0.30
Aspartic acid (3TMS)	152002	232_235 292_294 306_309	0.00 0.00 0.25
Pyroglutamic acid (2TMS)	153002	156_160 230_234 258_263	0.00 0.23 0.23
Glutamic acid (3TMS)	163001	246_250 128_131 230_234	0.23 0.00 0.23
Phenylalanine (2TMS)	164001	218_220 192_200 266_274	0.45 0.45 0.23
Asparagine (3TMS)	168001	116_118	0.00
Ornithine (3TMS)	176006	174_175 348_353	0.23 0.00
Ornithine (4TMS)	182002	142_146 174_175 420_425	0.00 0.23 0.00
Arginine (5TMS)	183001	157_161 256_261 373_379	0.25 0.20 0.43
Tyrosine (2TMS)	189006	179_186 91_98	0.25 0.71

Lysine (4TMS)	192003	156_161	1.67
		174_175	0.00
		317_322	0.27
Lysine (3TMS)	186002	174_175	0.00
		200_206	0.00
		258_264	0.00
Tyrosine (3TMS)	194002	218_220	0.58
		280_288	0.00
		354_362	0.00
Glycerol (3TMS)	129003	218_221	0.00
		263_265	0.20
		293_296	0.00
Fructose methoxyamine (5TMS)	187002	217_220	0.23
		307_310	0.45
Fructose methoxyamine {BP} (5TMS)	188004	307_310	0.96
		217_220	0.00
Mannose methoxyamine (5TMS)	188002	205_207	0.23
		217_220	0.00
		319_323	0.23
Glucose methoxyamine (5TMS)	189002	364_368	-0.06
		343_349	0.24
		291_294	0.00
Glucose methoxyamine {BP} (5TMS)	191001	364_368	1.12
		343_349	1.97
		291_294	1.39
Mannitol (6TMS)	193002	217_220	1.06
		319_323	0.00
Sorbitol (6TMS)	193001	217_220	0.00
		319_323	0.00
Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc	274002	451_457	3.32
		243_248	3.28
		435_441	3.32
Succinic acid (2TMS)	134001	247_251	0.18
		172_176	0.55
		248_252	0.67
Citramalic acid (3TMS)	148001	115_118	0.39
		247_251	0.39
		259_264	0.20
Malic acid (3TMS)	149001	233_236	0.00
		245_249	0.39
		335_339	0.18
Citric acid (4TMS)	182004	273_278	0.23

		347_352	0.23
		465_471	0.23
Glycerol-3-phosphate (4TMS)	177002	445_448	0.10
Fructose-6-phosphate methoxyamine (6TMS)	232002	217_220	0.00
		459_462	0.00
Glucose-6-phosphate methoxyamine (6TMS)	233002	471_475	-0.32
		160_162	0.32
[644; 2-Methyl-1,3-butanediol (2TMS)]	140003	117_119	0.00
		306_309	0.36
[700; 2-methyl-1,2-propanediol (2TMS)]	141003	131_134	0.00
		292_294	0.00
		277_279	0.36
[725; 2-Ketooctanoic acid (2TMS)]	146003	185_191	0.18
		212_219	0.36
		287_294	0.18
[545; 2,3-Dimethylsuccinic acid (2TMS)]	149003	291_298	0.18
		275_281	0.18
		207_209	0.18
[815; Ethyl-3(2H)-thiophenone]	150003	128_131	0.14
[729; N,N-Dimethyllysine methyl ester]	151003	128_131	0.71
		84_88	0.00
[680; 2,3-Dimethylsuccinic acid (2TMS)]	158003	287_294	0.45
		377_384	0.23
[882; Ornithine (3TMS)]	162001	142_146	0.00
		348_353	0.43
		115_117	0.00
[548; Leucine (2TBS)]	165002	315_320	0.00
		200_203	0.00
		330_335	-0.25
[612; 4-Aminobutyric acid (2TBS)]	175003	112_118	0.23
		274_280	0.25
		376_383	0.58
[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]	176005	184_189	0.23
[829; Orotic acid (3TMS)]	176003	254_258	0.25
		357_362	0.00
		269_274	-0.23
[757; 2-Desoxy-pentos-3-ylose dimethoxyamine (2TMS)]	176004	231_235	0.00
		315_321	0.61
[812; D-Xylofuranose (4TMS)]	177004	305_308	-0.15
[731; Erythrose (3TMS)]	184003	117_119	0.23

		217_220	0.23
		204_206	0.45
[826; beta-[[[(5-methyl-2-thienyl)methylene]amino]-benzeneacetic acid methyl ester]	187004	241_245	0.20
		431_437	0.00
		153_157	0.23
[772; D-Glucose (5TMS)]	189005	204_206	0.10
[793; D-Galactono-1,4-lactone (4TMS)]	196004	217_220	0.00
		243_248	0.00
		361_367	0.55
[945; beta-D-Glucopyranose (5TMS)]	197002	191_192	0.00
		204_206	0.00
		217_220	0.00
[775; Dopamine (4TMS)]	200002	174_175	0.00
		317_324	0.55
		375_382	0.55
[680; Glycerol-2-phosphate (4TMS)]	203004	243_248	0.58
		258_263	0.58
		169_174	0.85
[766; beta-D-Methylglucopyranoside (4TMS)]	203003	204_206	0.00
		259_264	0.00
		319_323	0.00
[607; Putrescine (4TMS)]	204003	375_379	-0.18
[756; beta-D-Methylglucopyranoside (4TMS)]	209004	204_206	0.27
		319_323	0.27
		243_248	0.55
[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]	211004	299_299	0.00
		315_315	0.00
[648; Ethylamine (2TMS)]	216002	174_175	0.00
		217_220	0.00
		345_349	-0.27
[705; 2-Ketogluconic acid (5TMS)]	217002	437_442	0.00
		257_262	0.00
		217_220	0.27
[733; Threitol (4TMS)]	218001	217_220	0.27
[715; Erythritol (4TMS)]	226001	373_382	0.46
		217_220	0.32
[945; Uridine (3TMS)]	248002	217_220	0.32
		259_264	0.32
[644; Erythritol (4TMS)]	252002	446_454	0.64
		217_220	0.00

[895; Isomaltose methoxyamine (8TMS)]	281001	204_206	0.32
		361_367	0.32
[542; Maltose methoxyamine {BP} (8TMS)]	282003	204_206	0.80

60

Table 3

NAME:13C_1731.2_1313EC11_Ribitol (5TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:173001-11-1
 RI:1731
 RT:10.550

NUM PEAKS: 41

(70	3)	(72	18)	(73	1000)	(74	80)	(75	63)
(87	8)	(89	7)	(90	22)	(103	32)	(104	189)
(105	13)	(106	5)	(119	83)	(131	28)	(132	120)
(133	70)	(134	12)	(146	11)	(147	318)	(148	50)
(149	30)	(191	50)	(192	20)	(206	53)	(207	98)
(208	18)	(209	6)	(220	215)	(221	71)	(222	20)
(223	4)	(248	15)	(279	9)	(280	4)	(281	4)
(310	23)	(311	6)	(322	8)	(323	42)	(324	12)
(325	5)								

NAME:13C_1318.4_1313EC16_Proline (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:132003-11-1

RI:1318

RT:6.620

NUM PEAKS: 19

(70	7)	(71	17)	(72	28)	(73	600)	(74	60)
(80	7)	(84	5)	(85	17)	(86	5)	(115	6)
(128	4)	(142	4)	(143	3)	(144	20)	(145	39)
(146	1000)	(147	90)	(148	33)	(220	38)		

NAME:13C_1318.9_1313EC16_Threonine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:132001-11-1

RI:1319

RT:6.627

NUM PEAKS: 58

(73	1000)	(75	547)	(76	49)	(77	23)	(79	8)
(81	58)	(82	5)	(88	115)	(89	29)	(90	4)
(91	3)	(92	3)	(93	7)	(96	4)	(102	45)
(103	54)	(104	22)	(105	15)	(106	4)	(114	3)
(116	11)	(117	80)	(118	56)	(119	667)	(120	55)
(121	21)	(129	2)	(130	7)	(132	40)	(133	663)
(134	170)	(135	38)	(136	6)	(149	335)	(150	30)
(151	12)	(153	3)	(159	5)	(161	7)	(162	31)
(178	4)	(190	2)	(191	2)	(192	2)	(205	7)
(206	17)	(207	10)	(208	3)	(210	2)	(221	193)
(222	33)	(223	27)	(224	5)	(225	3)	(234	5)
(235	3)	(252	18)	(253	3)				

NAME:13C_1413.9_1313EC16_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:141004-11-1

RI:1414

RT:7.745

NUM PEAKS: 27

(72	44)	(73	604)	(74	142)	(75	1000)	(76	120)
(77	113)	(87	85)	(88	70)	(103	47)	(104	71)
(105	62)	(106	26)	(117	85)	(118	29)	(119	145)
(120	39)	(121	447)	(132	323)	(133	198)	(148	76)
(151	59)	(160	25)	(161	22)	(162	190)	(163	21)
(164	15)	(177	23)						

NAME:13C_1420.9_1313EC16_Alanine (BP) (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:142001-11-1

RI:1421

RT:7.827

NUM PEAKS: 34

(72	122)	(73	1000)	(74	112)	(75	354)	(76	29)
(87	18)	(88	23)	(100	78)	(101	25)	(102	73)
(103	27)	(104	12)	(115	7)	(117	42)	(118	517)
(119	48)	(120	17)	(131	20)	(133	52)	(134	8)
(146	38)	(147	353)	(148	56)	(149	49)	(162	420)
(163	42)	(164	15)	(190	15)	(192	115)	(193	20)
(236	20)	(265	75)	(266	15)	(267	6)		

NAME:13C_1489.8_1313EC16_Malic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149001-11-1

RI:1490

RT:8.637

NUM PEAKS: 59

(70	3)	(72	30)	(73	1000)	(74	90)	(75	140)
(76	9)	(87	10)	(101	31)	(102	8)	(103	53)
(104	6)	(105	6)	(115	10)	(117	23)	(118	23)
(119	9)	(131	30)	(132	11)	(133	127)	(134	17)
(135	12)	(143	7)	(146	10)	(147	413)	(148	62)
(149	46)	(150	5)	(151	9)	(175	29)	(176	9)
(177	30)	(178	12)	(189	19)	(190	16)	(191	60)
(192	20)	(193	6)	(206	5)	(207	4)	(217	8)
(220	12)	(221	11)	(234	7)	(235	6)	(236	46)
(237	8)	(245	18)	(249	27)	(250	6)	(251	4)
(263	4)	(265	13)	(266	11)	(308	5)	(309	4)
(310	9)	(319	3)	(323	4)	(339	9)		

NAME:13C_1495.3_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150003-11-1

RI:1495

RT:8.703

NUM PEAKS: 52

(72	21)	(73	574)	(74	66)	(75	184)	(76	15)
(77	11)	(86	8)	(87	17)	(88	7)	(89	6)
(95	3)	(100	5)	(101	37)	(102	45)	(103	20)
(104	15)	(105	7)	(115	11)	(116	6)	(117	26)
(118	9)	(119	37)	(120	3)	(121	3)	(129	6)
(130	47)	(131	1000)	(132	133)	(133	81)	(134	10)
(135	3)	(146	3)	(147	74)	(148	12)	(149	14)
(160	9)	(161	5)	(162	11)	(176	4)	(177	6)
(193	96)	(194	8)	(195	3)	(204	16)	(205	51)
(206	12)	(207	4)	(220	9)	(221	3)	(234	12)
(296	4)	(311	3)						

NAME:13C_1521.6_1313EC16_Aspartic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152002-11-1

RI:1522

RT:8.925

NUM PEAKS: 74

(70	7)	(71	9)	(72	28)	(73	1000)	(74	104)
(75	156)	(76	11)	(77	8)	(84	3)	(85	6)
(86	7)	(87	13)	(88	4)	(89	5)	(100	13)
(101	93)	(102	157)	(103	26)	(104	15)	(105	4)

(115	6)	(116	7)	(117	17)	(118	23)	(119	40)
(120	4)	(121	5)	(130	5)	(131	28)	(132	42)
(133	52)	(134	11)	(135	7)	(145	17)	(146	10)
(147	157)	(148	28)	(149	26)	(150	4)	(162	3)
(163	21)	(164	4)	(173	3)	(174	7)	(175	11)
(176	9)	(178	5)	(189	3)	(190	44)	(191	11)
(192	5)	(203	3)	(204	40)	(205	11)	(206	13)
(207	4)	(218	4)	(219	21)	(220	71)	(221	18)
(222	7)	(233	4)	(234	20)	(235	357)	(236	64)
(237	30)	(238	4)	(248	4)	(249	3)	(294	5)
(309	10)	(310	3)	(338	5)	(353	3)		

NAME:13C_1594.8_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:159001-11-1

RI:1595

RT:9.493

NUM PEAKS: 33

(70	10)	(72	58)	(73	1000)	(74	105)	(75	173)
(86	10)	(87	21)	(100	20)	(101	51)	(102	30)
(115	14)	(117	40)	(118	15)	(131	20)	(133	37)
(139	12)	(144	17)	(145	36)	(146	575)	(147	211)
(148	48)	(174	9)	(175	15)	(189	15)	(190	388)
(191	40)	(192	14)	(220	128)	(221	21)	(222	9)
(293	36)	(294	8)	(295	4)				

NAME:13C_1630.8_1313EC16_Glutamic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:163001-11-1

RI:1631

RT:9.772

NUM PEAKS: 83

(70	7)	(71	9)	(72	28)	(73	1000)	(74	99)
(75	255)	(76	18)	(85	9)	(86	13)	(87	29)
(88	162)	(89	11)	(99	4)	(100	11)	(101	62)
(102	61)	(103	20)	(104	14)	(105	5)	(113	3)
(114	3)	(115	30)	(116	11)	(117	43)	(118	20)
(119	11)	(129	3)	(130	15)	(131	331)	(132	76)
(133	88)	(134	16)	(135	8)	(144	33)	(145	7)
(146	8)	(147	205)	(148	38)	(149	56)	(150	8)
(151	4)	(158	5)	(159	12)	(160	164)	(161	26)
(162	38)	(163	7)	(173	4)	(174	4)	(175	5)
(176	4)	(177	3)	(178	5)	(189	3)	(190	4)
(191	6)	(205	12)	(206	29)	(207	7)	(208	3)
(218	9)	(219	6)	(220	20)	(221	22)	(222	6)
(233	5)	(234	70)	(235	16)	(236	7)	(248	5)
(249	25)	(250	438)	(251	78)	(252	36)	(253	4)
(263	9)	(279	5)	(324	6)	(352	3)	(353	30)
(355	4)	(368	15)	(369	5)				

NAME:13C_1640.6_1313EC16_Phenylalanine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:164001-11-1

RI:1641

RT:9.848

NUM PEAKS: 69

(70	52)	(71	8)	(72	19)	(73	1000)	(74	93)
(75	105)	(76	6)	(83	12)	(86	6)	(87	20)
(96	12)	(97	17)	(98	163)	(99	14)	(100	5)
(101	171)	(104	9)	(110	3)	(111	13)	(112	3)

63

(113	3)	(117	8)	(118	5)	(119	5)	(124	3)
(125	6)	(126	10)	(127	11)	(128	12)	(132	59)
(133	33)	(134	7)	(135	3)	(138	5)	(139	8)
(140	6)	(141	6)	(145	4)	(146	4)	(147	156)
(148	30)	(149	13)	(153	3)	(154	3)	(155	3)
(159	3)	(161	4)	(163	9)	(168	13)	(169	4)
(170	5)	(175	4)	(184	9)	(185	9)	(198	3)
(199	23)	(200	267)	(201	24)	(202	8)	(205	8)
(213	10)	(219	10)	(220	377)	(221	82)	(222	33)
(223	5)	(274	23)	(275	7)	(303	6)		

NAME:13C_1707.8_1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:171003-11-1

RI:1708

RT:10.369

NUM PEAKS: 168

(70	4)	(71	26)	(72	27)	(73	1000)	(74	90)
(75	126)	(76	6)	(79	3)	(80	3)	(85	14)
(86	12)	(87	22)	(88	9)	(89	101)	(90	12)
(91	8)	(92	4)	(93	3)	(99	4)	(101	49)
(102	11)	(103	36)	(104	12)	(105	6)	(106	4)
(108	3)	(113	3)	(115	13)	(116	10)	(117	37)
(118	20)	(119	7)	(120	5)	(121	4)	(129	25)
(130	8)	(132	31)	(133	39)	(134	7)	(136	5)
(139	3)	(143	9)	(144	7)	(145	31)	(146	9)
(147	130)	(148	49)	(149	14)	(150	6)	(157	6)
(158	7)	(159	72)	(160	46)	(161	12)	(162	11)
(163	11)	(164	4)	(171	4)	(172	3)	(174	8)
(175	63)	(176	14)	(177	20)	(183	5)	(184	3)
(186	4)	(188	8)	(189	14)	(190	12)	(191	5)
(193	4)	(196	4)	(205	6)	(206	7)	(214	4)
(215	3)	(216	3)	(217	3)	(220	13)	(227	3)
(232	8)	(233	7)	(234	6)	(235	14)	(236	4)
(239	3)	(245	3)	(246	3)	(248	21)	(249	13)
(250	4)	(254	3)	(256	4)	(260	3)	(261	4)
(262	4)	(268	3)	(270	4)	(272	3)	(276	15)
(277	28)	(278	15)	(279	105)	(280	21)	(285	3)
(286	6)	(290	3)	(291	3)	(292	7)	(293	4)
(298	5)	(299	5)	(300	4)	(306	5)	(307	10)
(308	6)	(309	5)	(314	5)	(315	3)	(316	3)
(320	5)	(321	11)	(322	7)	(328	3)	(338	4)
(340	3)	(342	3)	(344	3)	(346	4)	(349	3)
(351	8)	(367	4)	(368	3)	(370	3)	(376	4)
(378	3)	(379	4)	(380	5)	(398	3)	(400	3)
(401	4)	(404	3)	(409	3)	(425	3)	(429	4)
(438	3)	(449	4)	(450	3)	(456	4)	(457	4)
(475	3)	(480	5)	(481	3)	(483	3)	(484	3)
(487	6)	(488	3)	(505	3)	(506	3)	(510	4)
(514	3)	(519	3)	(523	3)	(531	3)	(534	4)
(536	3)	(537	3)	(543	4)				

NAME:13C_1720.2_1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:172005-11-1

RI:1720

RT:10.465

NUM PEAKS: 47

(72	28)	(73	767)	(74	167)	(75	1000)	(76	86)
(77	40)	(78	9)	(86	16)	(87	224)	(88	272)

64

(90 186) (91 21) (92 6) (101 36) (116 9)
 (117 111) (118 155) (131 56) (133 189) (134 15)
 (135 6) (143 64) (144 35) (145 9) (146 20)
 (148 72) (149 39) (151 5) (159 269) (160 555)
 (161 142) (162 121) (163 37) (164 9) (173 7)
 (175 5) (176 53) (177 668) (178 59) (179 31)
 (205 11) (223 14) (233 71) (234 26) (235 11)
 (279 3) (280 26)

NAME:13C_1746.9_1313EC16_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:175003-11-1
 RI:1747
 RT:10.672

NUM PEAKS: 13

(72 35) (73 1000) (74 98) (75 217) (88 144)
 (89 106) (117 50) (118 371) (147 203) (190 40)
 (221 108) (280 293) (281 49)

NAME:13C_1769.9_1313EC16_Glycerol-3-phosphate (4TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:177002-11-1
 RI:1770
 RT:10.850

NUM PEAKS: 108

(70 5) (72 26) (73 1000) (74 87) (75 119)
 (76 8) (77 18) (79 3) (90 9) (91 5)
 (98 3) (102 14) (103 109) (104 98) (105 25)
 (106 5) (107 5) (115 17) (116 20) (117 11)
 (118 32) (119 25) (120 4) (121 8) (123 3)
 (131 23) (132 74) (133 123) (134 52) (135 37)
 (136 5) (137 13) (147 150) (148 24) (149 21)
 (150 3) (151 10) (153 3) (163 3) (164 5)
 (165 5) (167 4) (179 4) (181 18) (182 3)
 (183 6) (193 20) (194 4) (195 18) (196 3)
 (197 5) (205 3) (206 13) (207 39) (208 9)
 (209 6) (210 4) (211 97) (212 15) (213 9)
 (223 3) (225 20) (226 7) (227 18) (228 3)
 (242 17) (243 12) (255 8) (256 3) (257 19)
 (258 3) (269 4) (283 5) (284 3) (285 20)
 (286 5) (298 17) (299 180) (300 49) (301 25)
 (302 4) (313 3) (314 12) (315 44) (316 13)
 (317 6) (329 12) (330 4) (343 13) (344 6)
 (345 3) (358 19) (359 113) (360 34) (361 16)
 (362 3) (372 5) (373 30) (374 10) (375 5)
 (386 3) (387 12) (388 5) (389 5) (447 4)
 (448 17) (449 7) (450 3)

NAME:13C_1771.0_1313EC16_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:177003-11-1
 RI:1771
 RT:10.859

NUM PEAKS: 41

(83 83) (87 766) (101 497) (111 47) (112 24)
 (129 41) (130 121) (143 46) (159 137) (160 296)
 (172 89) (173 999) (174 192) (175 1000) (176 159)
 (187 117) (188 76) (201 93) (202 342) (203 62)
 (216 111) (217 73) (248 155) (250 28) (260 38)
 (294 27) (305 25) (306 28) (333 30) (334 204)

65

(335 247) (336 98) (340 19) (350 182) (351 59)
 (366 39) (411 26) (426 18) (514 20) (536 21)
 (540 17)

NAME:13C_1784.2_1313EC16_Glutamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:178001-11-1

RI:1784

RT:10.961

NUM PEAKS: 88

(70 11) (71 17) (72 32) (73 1000) (74 139)
 (75 301) (76 22) (77 12) (84 4) (85 23)
 (86 13) (87 52) (88 14) (89 7) (90 5)
 (99 5) (100 9) (101 46) (102 33) (103 13)
 (105 3) (113 4) (114 3) (115 28) (116 32)
 (117 64) (118 33) (119 9) (129 13) (130 12)
 (131 97) (132 43) (133 111) (134 15) (135 7)
 (142 3) (143 49) (144 20) (145 11) (146 22)
 (147 164) (148 67) (149 37) (150 6) (157 5)
 (158 17) (159 262) (160 744) (161 87) (162 32)
 (163 3) (172 4) (173 3) (174 6) (175 5)
 (176 3) (177 8) (188 3) (189 6) (190 13)
 (191 4) (203 3) (204 3) (205 67) (206 15)
 (207 6) (217 4) (218 4) (219 9) (220 19)
 (221 10) (231 7) (232 5) (233 27) (234 15)
 (235 12) (248 9) (249 94) (250 17) (251 7)
 (262 6) (263 3) (277 5) (278 7) (305 7)
 (352 15) (353 5) (367 5)

NAME:13C_1821.6_1313EC16_Ornithine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182002-11-1

RI:1822

RT:11.252

NUM PEAKS: 70

(73 736) (74 117) (85 13) (86 15) (87 130)
 (88 16) (89 6) (90 6) (100 18) (101 85)
 (102 54) (103 54) (104 17) (105 3) (113 6)
 (114 14) (115 25) (116 26) (117 41) (128 4)
 (129 9) (130 81) (131 77) (132 32) (144 19)
 (145 41) (146 1000) (157 8) (158 7) (159 12)
 (160 8) (161 11) (162 4) (172 3) (173 33)
 (174 33) (175 333) (176 61) (177 35) (178 5)
 (189 10) (190 15) (191 11) (192 8) (202 7)
 (203 70) (204 19) (205 20) (206 16) (218 38)
 (219 16) (220 54) (236 3) (246 7) (247 6)
 (248 3) (249 7) (263 28) (264 27) (265 6)
 (290 3) (320 6) (321 4) (335 9) (336 3)
 (410 3) (424 4) (425 23) (426 10) (427 5)

NAME:13C_1829.5_1313EC16_Arginine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:183001-11-1

RI:1830

RT:11.313

NUM PEAKS: 91

(70 25) (71 20) (72 126) (73 1000) (74 244)
 (75 99) (76 7) (84 6) (85 76) (86 27)
 (87 34) (88 13) (89 11) (90 13) (98 3)
 (99 11) (100 73) (101 58) (102 55) (103 16)

66

(104	14)	(113	4)	(114	6)	(115	21)	(116	14)
(117	57)	(118	14)	(123	5)	(128	13)	(129	32)
(130	22)	(131	50)	(132	36)	(133	33)	(134	6)
(142	4)	(143	18)	(144	42)	(145	105)	(146	201)
(147	110)	(148	35)	(149	10)	(156	4)	(157	9)
(158	14)	(159	46)	(160	60)	(161	521)	(162	59)
(163	20)	(171	4)	(172	35)	(173	37)	(174	16)
(177	9)	(187	3)	(188	14)	(189	9)	(190	10)
(191	5)	(192	6)	(201	3)	(202	3)	(203	3)
(204	4)	(205	3)	(217	3)	(218	3)	(219	17)
(220	29)	(221	6)	(222	3)	(234	3)	(235	5)
(245	8)	(246	4)	(248	4)	(249	18)	(250	3)
(259	4)	(260	15)	(261	189)	(262	37)	(263	16)
(264	6)	(274	4)	(289	3)	(335	3)	(364	5)
(379	7)								

NAME:13C_1835.5_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184003-11-1

RI:1836

RT:11.359

NUM PEAKS: 91

(71	8)	(72	27)	(73	1000)	(74	86)	(75	140)
(76	11)	(77	9)	(86	13)	(87	45)	(88	75)
(89	12)	(90	37)	(91	4)	(101	21)	(102	20)
(103	39)	(104	73)	(105	17)	(106	3)	(114	12)
(115	14)	(116	30)	(117	21)	(118	38)	(119	123)
(120	11)	(121	4)	(129	4)	(130	7)	(131	40)
(132	78)	(133	97)	(134	21)	(135	10)	(143	5)
(146	18)	(147	251)	(148	42)	(149	44)	(150	6)
(151	3)	(157	3)	(158	4)	(160	44)	(162	23)
(163	16)	(164	16)	(165	3)	(175	28)	(176	13)
(177	27)	(178	10)	(179	4)	(188	11)	(189	13)
(190	5)	(191	45)	(192	65)	(193	13)	(194	4)
(202	3)	(203	8)	(204	21)	(205	6)	(206	87)
(207	37)	(208	9)	(217	8)	(218	12)	(219	6)
(220	87)	(221	72)	(222	17)	(223	5)	(232	10)
(233	51)	(234	14)	(235	41)	(236	24)	(237	7)
(250	8)	(263	3)	(278	4)	(279	3)	(307	8)
(322	12)	(323	10)	(324	4)	(337	20)	(338	4)
(412	4)								

NAME:13C_1843.2_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184004-11-1

RI:1843

RT:11.419

NUM PEAKS: 29

(72	23)	(73	1000)	(74	79)	(75	100)	(89	6)
(90	16)	(102	10)	(103	40)	(104	57)	(115	9)
(118	21)	(119	59)	(131	26)	(132	62)	(133	64)
(134	13)	(147	221)	(148	39)	(149	25)	(191	44)
(192	259)	(193	43)	(194	17)	(206	349)	(207	66)
(208	24)	(220	129)	(222	12)	(235	5)		

NAME:13C_1870.4_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187004-11-1

RI:1870

RT:11.629

67

NUM PEAKS: 85

(70 10) (71 11) (72 21) (73 1000) (74 88)
 (75 68) (76 3) (84 5) (85 15) (86 5)
 (87 7) (90 9) (98 4) (99 8) (100 17)
 (101 8) (102 6) (103 19) (104 27) (105 4)
 (113 4) (114 3) (115 6) (117 6) (118 5)
 (119 21) (127 7) (128 7) (129 6) (130 5)
 (131 20) (133 46) (134 7) (135 4) (141 3)
 (142 4) (143 8) (144 4) (145 3) (147 111)
 (148 18) (149 12) (155 6) (156 11) (157 84)
 (158 15) (159 8) (170 7) (171 41) (172 25)
 (173 31) (175 3) (177 6) (185 5) (186 10)
 (187 4) (200 5) (201 9) (202 3) (206 12)
 (213 4) (214 6) (215 9) (216 3) (229 4)
 (230 11) (231 5) (243 6) (244 82) (245 658)
 (246 137) (247 56) (248 7) (273 11) (274 3)
 (275 3) (318 3) (319 5) (347 3) (348 3)
 (362 4) (436 3) (437 12) (438 5) (452 3)

NAME:13C_1879.2_1313EC16_Adenine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188005-11-1

RI:1879

RT:11.698

NUM PEAKS: 8

(73 800) (74 88) (197 207) (268 190) (269 1000)
 (270 172) (283 51) (284 190)

NAME:13C_1892.4_1313EC16_Tyrosine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189006-11-1

RI:1892

RT:11.800

NUM PEAKS: 102

(70 22) (75 321) (76 26) (77 18) (79 3)
 (80 3) (81 7) (82 13) (83 30) (84 29)
 (85 25) (88 29) (91 8) (92 5) (93 4)
 (94 3) (95 7) (96 33) (97 34) (98 56)
 (99 11) (100 10) (109 5) (110 13) (111 14)
 (112 16) (113 11) (114 11) (118 13) (123 7)
 (124 7) (125 19) (126 28) (127 42) (128 8)
 (129 6) (137 4) (138 9) (139 7) (140 14)
 (141 28) (142 10) (143 9) (151 4) (152 9)
 (153 5) (155 19) (156 42) (157 20) (158 5)
 (166 3) (167 4) (168 9) (169 11) (170 34)
 (171 15) (172 32) (173 6) (180 3) (183 14)
 (184 25) (185 71) (186 1000) (187 144) (188 36)
 (197 3) (198 6) (199 6) (200 19) (201 5)
 (202 3) (203 5) (212 3) (213 3) (214 8)
 (215 26) (216 102) (217 12) (221 48) (223 5)
 (226 3) (227 12) (228 5) (229 4) (231 3)
 (245 4) (260 3) (264 3) (272 3) (273 4)
 (290 3) (295 3) (296 3) (301 7) (302 5)
 (307 3) (317 3) (318 5) (319 32) (320 7)
 (321 5) (334 4)

NAME:13C_1940.3_1313EC16_Tyrosine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:194002-11-1

RI:1940

68

RT:12.115

NUM PEAKS: 99

(70	8)	(71	6)	(72	19)	(73	1000)	(74	91)
(75	113)	(76	7)	(77	4)	(82	3)	(83	7)
(84	6)	(85	7)	(86	4)	(87	17)	(88	3)
(96	10)	(97	11)	(98	15)	(99	3)	(100	4)
(101	167)	(102	27)	(103	12)	(104	7)	(110	5)
(111	5)	(112	7)	(113	3)	(114	3)	(115	3)
(116	4)	(117	6)	(118	4)	(119	3)	(124	3)
(125	5)	(126	6)	(127	4)	(130	3)	(131	15)
(132	52)	(133	25)	(134	6)	(137	3)	(138	4)
(139	3)	(140	5)	(141	10)	(142	3)	(145	3)
(146	4)	(147	109)	(148	19)	(149	10)	(152	4)
(153	3)	(154	6)	(155	7)	(156	19)	(157	4)
(158	3)	(159	3)	(160	4)	(161	5)	(163	9)
(168	5)	(169	4)	(170	15)	(171	8)	(172	9)
(175	4)	(182	3)	(183	5)	(184	10)	(185	8)
(186	69)	(187	10)	(188	4)	(198	3)	(199	4)
(200	16)	(201	3)	(205	6)	(214	3)	(215	8)
(219	14)	(220	594)	(221	105)	(222	50)	(223	5)
(273	7)	(287	9)	(288	55)	(289	10)	(290	4)
(362	13)	(363	6)	(364	3)	(391	6)		

NAME:13C_1294.2_1313EC11_Glycerol (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129003-11-1

RI:1294

RT:6.336

NUM PEAKS: 46

(70	4)	(71	6)	(72	26)	(73	1000)	(74	89)
(75	84)	(76	6)	(87	15)	(88	7)	(89	19)
(90	45)	(101	6)	(102	14)	(103	82)	(104	365)
(105	39)	(106	14)	(118	41)	(119	384)	(120	31)
(132	83)	(134	45)	(147	644)	(148	102)	(149	71)
(150	9)	(160	4)	(161	4)	(164	11)	(175	5)
(176	5)	(177	71)	(178	42)	(179	11)	(180	3)
(192	31)	(206	71)	(207	276)	(208	61)	(209	26)
(220	24)	(221	133)	(222	26)	(223	12)	(265	3)
(296	18)								

NAME:13C_1326.8_1313EC11_Glycine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:133001-11-1

RI:1327

RT:6.720

NUM PEAKS: 59

(70	12)	(71	9)	(72	26)	(73	1000)	(74	86)
(75	61)	(86	14)	(87	313)	(88	26)	(89	14)
(99	5)	(100	23)	(101	171)	(102	32)	(103	32)
(104	5)	(105	5)	(113	7)	(114	5)	(115	11)
(116	18)	(117	52)	(118	12)	(119	13)	(129	3)
(130	44)	(131	52)	(132	15)	(133	163)	(134	23)
(135	12)	(147	310)	(148	50)	(149	24)	(159	25)
(160	14)	(161	16)	(162	3)	(173	11)	(174	15)
(175	905)	(176	161)	(177	73)	(178	14)	(188	3)
(190	14)	(191	3)	(204	11)	(205	3)	(206	3)
(247	9)	(248	6)	(249	144)	(250	39)	(251	18)
(252	3)	(278	44)	(279	11)	(280	6)		

NAME:13C_1340.7_1313EC11_Succinic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:134001-11-1

RI:1341

RT:6.883

NUM PEAKS: 25

(72	25)	(73	546)	(74	56)	(75	378)	(76	27)
(87	13)	(88	12)	(89	9)	(103	13)	(115	8)
(116	8)	(117	9)	(118	25)	(131	22)	(132	95)
(133	51)	(134	11)	(147	1000)	(148	159)	(149	84)
(176	43)	(177	20)	(179	7)	(251	75)	(252	11)

NAME:13C_1380.4_1313EC11_Alanine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138002-11-1

RI:1380

RT:7.350

NUM PEAKS: 50

(70	25)	(71	27)	(72	36)	(73	999)	(85	23)
(86	22)	(99	10)	(100	47)	(102	790)	(103	93)
(113	12)	(114	10)	(116	233)	(117	68)	(129	6)
(130	72)	(131	95)	(133	261)	(135	18)	(139	3)
(144	6)	(147	370)	(148	35)	(158	6)	(159	28)
(160	10)	(161	9)	(173	24)	(174	28)	(176	25)
(177	6)	(187	3)	(188	7)	(189	26)	(190	1000)
(191	181)	(192	81)	(193	24)	(203	5)	(233	4)
(247	11)	(248	4)	(263	6)	(264	137)	(265	38)
(266	17)	(292	3)	(293	28)	(294	8)	(295	4)

NAME:13C_1381.6_1313EC11_Serine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138001-11-1

RI:1382

RT:7.365

NUM PEAKS: 58

(70	7)	(71	10)	(72	27)	(73	1000)	(74	104)
(75	158)	(76	11)	(77	6)	(85	8)	(86	7)
(87	22)	(88	11)	(89	19)	(90	9)	(100	10)
(101	122)	(103	22)	(104	63)	(105	10)	(106	3)
(115	14)	(117	25)	(118	70)	(119	26)	(120	4)
(131	29)	(132	46)	(133	73)	(134	24)	(135	8)
(145	7)	(146	11)	(147	163)	(148	31)	(150	6)
(159	5)	(160	7)	(161	5)	(162	6)	(163	7)
(174	9)	(175	10)	(176	9)	(177	5)	(204	7)
(205	28)	(206	318)	(207	57)	(208	25)	(218	3)
(219	16)	(220	169)	(221	37)	(222	15)	(223	3)
(280	17)	(281	5)	(309	8)				

NAME:13C_1405.3_1313EC11_Threonine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140001-11-1

RI:1405

RT:7.644

NUM PEAKS: 71

(70	6)	(71	8)	(72	27)	(73	1000)	(74	100)
(75	135)	(76	9)	(77	5)	(85	7)	(86	6)
(87	28)	(88	23)	(89	9)	(99	3)	(100	5)
(101	93)	(102	167)	(103	43)	(104	18)	(105	7)
(115	12)	(116	7)	(117	45)	(118	20)	(119	219)
(120	19)	(121	8)	(130	13)	(131	141)	(132	73)
(133	92)	(134	30)	(135	9)	(145	8)	(146	7)

70

(147 153) (148 30) (149 23) (150 3) (159 6)
 (160 16) (161 14) (162 6) (163 6) (173 4)
 (175 8) (176 3) (177 3) (178 5) (189 7)
 (190 3) (191 5) (192 7) (204 3) (205 51)
 (206 17) (207 8) (219 5) (220 86) (221 309)
 (222 60) (223 26) (224 3) (234 6) (292 3)
 (293 53) (294 16) (295 30) (296 8) (297 3)
 (324 9)

NAME:13C_1411.1_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:141003-11-1
 RI:1411
 RT:7.711

NUM PEAKS: 27
 (71 217) (73 785) (74 54) (81 73) (85 65)
 (95 18) (99 9) (103 88) (110 27) (118 46)
 (133 129) (134 1000) (135 90) (136 21) (147 231)
 (148 38) (149 62) (150 9) (157 6) (191 18)
 (192 16) (207 10) (279 9) (280 7) (294 126)
 (295 28) (296 14)

NAME:13C_1440.4_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:144003-11-1
 RI:1440
 RT:8.056

NUM PEAKS: 54
 (70 8) (71 9) (72 33) (73 1000) (74 143)
 (75 437) (76 41) (77 20) (85 6) (86 6)
 (87 16) (88 12) (89 12) (90 3) (91 6)
 (100 5) (101 13) (102 67) (103 23) (104 27)
 (105 4) (115 6) (116 7) (117 20) (118 262)
 (119 143) (120 18) (121 4) (131 31) (132 279)
 (133 59) (134 17) (146 7) (147 171) (148 46)
 (149 22) (150 4) (161 4) (162 39) (163 455)
 (164 40) (165 17) (175 6) (176 8) (191 5)
 (204 16) (205 3) (222 13) (237 29) (238 5)
 (248 8) (249 38) (250 6) (266 10)

NAME:13C_1458.8_1313EC11_Homoserine (3TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:146001-11-1
 RI:1459
 RT:8.273

NUM PEAKS: 67
 (70 8) (71 11) (72 31) (73 1000) (74 103)
 (75 145) (76 12) (85 9) (86 7) (87 23)
 (88 17) (89 10) (90 4) (95 3) (100 13)
 (101 44) (102 83) (103 69) (104 223) (105 30)
 (106 10) (113 3) (115 15) (116 11) (117 25)
 (118 15) (119 9) (129 5) (130 23) (131 399)
 (132 77) (133 112) (134 37) (135 9) (144 4)
 (145 6) (146 7) (147 141) (148 28) (149 48)
 (150 6) (159 4) (160 9) (161 6) (173 3)
 (175 6) (176 17) (177 9) (189 3) (190 7)
 (192 4) (204 7) (205 32) (206 8) (218 7)
 (219 12) (220 42) (221 487) (222 84) (223 37)
 (224 4) (234 22) (235 6) (236 7) (295 15)
 (296 5) (324 7)

NAME:13C_1464.4_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146003-11-1

RI:1464

RT:8.339

NUM PEAKS: 50

(70	22)	(71	24)	(72	83)	(73	580)	(75	242)
(76	18)	(77	19)	(83	4)	(84	7)	(85	32)
(86	46)	(87	10)	(88	5)	(89	4)	(99	8)
(100	22)	(101	44)	(105	4)	(113	5)	(114	5)
(115	14)	(116	7)	(129	24)	(130	14)	(133	60)
(134	9)	(135	5)	(147	1000)	(148	161)	(149	97)
(150	10)	(151	3)	(159	13)	(160	6)	(173	12)
(175	8)	(190	11)	(191	32)	(192	3)	(203	7)
(218	8)	(219	68)	(220	16)	(221	3)	(263	7)
(264	4)	(293	9)	(294	70)	(295	12)	(296	4)

NAME:13C_1467.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147003-11-1

RI:1467

RT:8.372

NUM PEAKS: 57

(71	42)	(73	1000)	(74	100)	(80	7)	(81	3)
(82	4)	(87	49)	(88	17)	(89	15)	(90	7)
(99	9)	(100	43)	(101	99)	(102	268)	(103	49)
(104	15)	(109	3)	(114	14)	(115	34)	(116	27)
(117	412)	(118	43)	(119	20)	(128	7)	(130	60)
(131	667)	(132	92)	(142	15)	(143	11)	(144	34)
(145	307)	(146	57)	(154	11)	(157	11)	(158	57)
(159	26)	(160	13)	(161	5)	(162	5)	(172	9)
(174	185)	(175	25)	(176	18)	(188	3)	(189	9)
(205	20)	(216	2)	(217	3)	(232	9)	(233	3)
(246	8)	(247	17)	(248	188)	(249	32)	(250	13)
(262	5)	(263	16)						

NAME:13C_1473.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147002-11-1

RI:1473

RT:8.442

NUM PEAKS: 64

(74	1000)	(77	3)	(78	3)	(80	3)	(85	6)
(86	7)	(87	5)	(88	7)	(89	6)	(90	50)
(91	5)	(94	4)	(101	40)	(102	25)	(105	3)
(110	3)	(114	3)	(115	4)	(116	4)	(117	32)
(122	3)	(130	5)	(131	10)	(132	36)	(142	4)
(145	8)	(146	146)	(157	3)	(158	7)	(159	5)
(160	4)	(162	5)	(163	37)	(164	7)	(174	10)
(176	23)	(186	3)	(188	5)	(191	5)	(194	4)
(210	3)	(215	3)	(220	14)	(228	3)	(245	3)
(280	4)	(323	3)	(335	4)	(349	3)	(360	3)
(385	3)	(386	4)	(387	3)	(410	3)	(423	3)
(431	4)	(434	3)	(441	3)	(459	3)	(495	3)
(524	4)	(532	3)	(535	3)	(542	3)		

NAME:13C_1481.0_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148002-11-1

RI:1481

RT:8.534

NUM PEAKS: 16

(71	19)	(73	1000)	(85	62)	(87	47)	(101	44)
(102	59)	(103	15)	(104	31)	(143	143)	(147	273)
(149	21)	(158	34)	(159	985)	(160	91)	(161	30)
(233	55)								

NAME:13C_1503.6_1313EC11_Erythritol (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150002-11-1

RI:1504

RT:8.786

NUM PEAKS: 56

(73	1000)	(74	74)	(75	50)	(76	3)	(87	4)
(89	11)	(90	29)	(103	54)	(104	186)	(105	20)
(106	5)	(115	5)	(116	7)	(119	154)	(120	11)
(121	5)	(131	16)	(132	68)	(133	94)	(134	15)
(135	8)	(145	3)	(146	5)	(147	347)	(148	55)
(149	33)	(150	3)	(177	6)	(178	3)	(189	3)
(191	67)	(192	56)	(193	12)	(194	3)	(205	4)
(206	72)	(207	114)	(208	22)	(209	8)	(218	3)
(219	12)	(220	220)	(221	53)	(222	19)	(223	3)
(235	7)	(279	6)	(280	3)	(295	12)	(296	4)
(309	5)	(310	17)	(311	5)	(312	3)	(324	6)
(325	3)								

NAME:13C_1506.4_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151002-11-1

RI:1506

RT:8.808

NUM PEAKS: 68

(75	501)	(76	44)	(87	77)	(93	13)	(101	233)
(102	965)	(115	44)	(116	44)	(117	1000)	(122	8)
(123	16)	(130	46)	(131	727)	(145	50)	(157	24)
(158	28)	(159	114)	(161	10)	(185	36)	(186	16)
(190	15)	(197	17)	(199	12)	(203	73)	(204	35)
(210	10)	(218	20)	(227	17)	(235	18)	(238	14)
(242	11)	(243	20)	(244	9)	(246	48)	(247	434)
(248	74)	(249	20)	(250	8)	(269	13)	(270	12)
(275	24)	(276	15)	(281	13)	(282	22)	(305	10)
(313	10)	(325	10)	(339	10)	(346	16)	(347	11)
(350	14)	(356	10)	(360	13)	(361	9)	(368	7)
(376	11)	(405	14)	(426	8)	(436	9)	(440	10)
(448	9)	(453	12)	(454	17)	(464	10)	(518	10)
(524	7)	(542	10)	(553	6)				

NAME:13C_1513.8_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151003-11-1

RI:1514

RT:8.865

NUM PEAKS: 67

(70	12)	(72	37)	(73	1000)	(74	116)	(75	276)
(76	21)	(77	12)	(85	14)	(86	26)	(87	59)
(88	909)	(89	209)	(90	21)	(91	15)	(100	14)
(101	79)	(102	147)	(103	23)	(104	28)	(105	32)
(106	5)	(114	4)	(115	18)	(116	8)	(117	49)
(118	17)	(119	10)	(120	19)	(130	7)	(131	102)

73

(132	53)	(133	60)	(134	11)	(135	5)	(144	46)
(145	10)	(146	13)	(147	159)	(148	36)	(149	17)
(158	7)	(159	7)	(160	118)	(161	18)	(162	38)
(163	17)	(174	8)	(175	5)	(176	27)	(177	5)
(190	9)	(191	55)	(192	885)	(193	87)	(194	34)
(205	22)	(206	7)	(218	4)	(219	3)	(220	17)
(221	7)	(234	31)	(266	14)	(279	23)	(280	4)
(295	10)	(310	10)						

NAME:13C_1528.8_1313EC11_Pyroglutamic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:153002-11-1

RI:1529

RT:8.981

NUM PEAKS: 56

(70	20)	(71	33)	(72	36)	(73	955)	(75	138)
(76	9)	(77	5)	(84	7)	(85	27)	(86	24)
(87	21)	(88	24)	(95	7)	(99	5)	(100	7)
(101	24)	(104	4)	(105	4)	(113	6)	(114	4)
(115	31)	(116	8)	(117	25)	(118	6)	(124	14)
(130	5)	(131	22)	(132	9)	(133	38)	(134	6)
(135	3)	(143	4)	(144	29)	(145	11)	(147	167)
(148	27)	(149	17)	(157	3)	(158	16)	(159	42)
(160	1000)	(161	89)	(162	38)	(173	4)	(191	4)
(218	12)	(232	4)	(233	4)	(234	83)	(235	14)
(236	6)	(262	6)	(263	72)	(264	12)	(265	6)
(278	3)								

NAME:13C_1537.7_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154002-11-1

RI:1538

RT:9.050

NUM PEAKS: 66

(72	26)	(73	543)	(74	85)	(75	685)	(76	58)
(77	35)	(86	15)	(87	66)	(88	1000)	(89	26)
(90	6)	(91	6)	(100	6)	(101	10)	(102	10)
(103	26)	(104	22)	(105	5)	(115	13)	(116	6)
(117	14)	(118	44)	(119	21)	(120	3)	(131	17)
(132	47)	(133	58)	(134	13)	(135	5)	(143	3)
(144	45)	(145	7)	(146	14)	(147	81)	(148	44)
(149	25)	(150	4)	(158	3)	(159	4)	(160	76)
(161	24)	(162	225)	(163	24)	(164	10)	(176	8)
(177	39)	(178	440)	(179	41)	(180	17)	(190	8)
(191	78)	(192	6)	(193	3)	(206	21)	(207	3)
(218	3)	(234	43)	(235	8)	(236	4)	(252	17)
(253	3)	(263	6)	(280	3)	(281	39)	(282	7)
(283	3)								

NAME:13C_1561.1_1313EC11_Phenylalanine (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157001-11-1

RI:1561

RT:9.232

NUM PEAKS: 85

(70	121)	(72	29)	(73	590)	(74	118)	(75	345)
(76	35)	(77	17)	(81	9)	(83	87)	(87	31)
(89	22)	(91	36)	(92	5)	(96	25)	(97	29)
(98	260)	(99	31)	(100	33)	(101	39)	(102	16)
(104	38)	(108	4)	(110	17)	(111	101)	(113	7)

(116	7)	(118	28)	(121	3)	(124	5)	(125	15)
(126	44)	(127	106)	(128	1000)	(129	4)	(132	186)
(133	42)	(134	19)	(138	3)	(139	18)	(140	5)
(143	9)	(145	5)	(148	414)	(149	40)	(150	22)
(154	4)	(158	4)	(159	63)	(161	7)	(169	9)
(174	3)	(175	14)	(177	4)	(184	13)	(185	13)
(200	3)	(202	8)	(213	33)	(214	6)	(218	4)
(220	56)	(221	15)	(222	63)	(223	9)	(224	5)
(230	3)	(231	19)	(232	3)	(235	3)	(237	4)
(244	3)	(251	7)	(286	3)	(296	3)	(303	3)
(304	3)	(396	5)	(397	4)	(403	3)	(449	3)
(470	3)	(500	3)	(506	3)	(544	3)	(565	3)

NAME:13C 1575.2 1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157002-11-1

RI:1575

RT:9.341

NUM PEAKS: 57

(72	34)	(73	1000)	(74	121)	(75	221)	(76	16)
(77	8)	(86	3)	(89	7)	(102	8)	(103	39)
(105	6)	(111	5)	(115	6)	(118	29)	(119	11)
(131	25)	(132	9)	(133	75)	(134	10)	(135	6)
(145	5)	(146	52)	(147	430)	(148	119)	(149	87)
(150	12)	(151	5)	(161	6)	(162	62)	(163	9)
(175	8)	(176	3)	(177	4)	(178	13)	(191	10)
(192	109)	(193	19)	(194	7)	(207	4)	(221	19)
(222	13)	(235	4)	(236	35)	(237	6)	(266	27)
(267	8)	(280	7)	(281	89)	(282	16)	(283	6)
(294	8)	(308	6)	(310	8)	(355	4)	(383	3)
(384	12)	(385	5)						

NAME:13C 1580.5 1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158002-11-1

RI:1581

RT:9.382

NUM PEAKS: 104

(109	37)	(110	25)	(111	46)	(112	30)	(122	61)
(123	71)	(124	68)	(125	82)	(126	60)	(127	104)
(128	25)	(185	88)	(186	1000)	(187	69)	(201	90)
(271	13)	(273	13)	(274	22)	(275	84)	(276	11)
(287	20)	(289	11)	(290	89)	(291	20)	(346	12)
(347	17)	(360	14)	(362	24)	(363	18)	(364	28)
(365	31)	(366	12)	(371	19)	(379	10)	(392	14)
(398	19)	(402	20)	(437	15)	(438	18)	(439	19)
(440	12)	(441	19)	(442	16)	(445	22)	(446	11)
(447	25)	(448	10)	(449	19)	(450	40)	(451	27)
(455	31)	(456	21)	(457	29)	(458	29)	(459	30)
(461	39)	(463	27)	(464	23)	(465	27)	(466	30)
(467	38)	(469	29)	(470	25)	(471	20)	(472	24)
(473	43)	(474	32)	(476	28)	(477	16)	(478	29)
(479	17)	(480	18)	(482	31)	(483	18)	(486	21)
(488	26)	(489	20)	(492	18)	(493	12)	(495	26)
(496	33)	(498	20)	(500	17)	(502	14)	(503	13)
(504	27)	(505	22)	(510	15)	(513	15)	(514	29)
(515	20)	(517	18)	(527	15)	(529	16)	(532	21)
(533	14)	(538	14)	(540	17)	(542	20)	(543	16)
(548	17)	(549	21)	(555	14)	(558	10)		

75

NAME:13C_1581.9_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158003-11-1

RI:1582

RT:9.393

NUM PEAKS: 86

(70	8)	(71	9)	(72	48)	(73	1000)	(74	160)
(75	299)	(76	16)	(85	4)	(86	6)	(87	9)
(91	25)	(100	3)	(101	22)	(102	9)	(103	28)
(104	5)	(105	4)	(115	8)	(116	3)	(117	49)
(118	42)	(119	45)	(130	8)	(131	33)	(133	100)
(134	14)	(135	9)	(145	4)	(146	17)	(147	386)
(148	86)	(149	84)	(150	12)	(151	5)	(161	7)
(162	70)	(163	20)	(164	5)	(175	15)	(176	5)
(177	8)	(178	3)	(190	3)	(191	40)	(192	12)
(193	6)	(204	3)	(205	3)	(206	7)	(207	9)
(219	6)	(220	51)	(221	32)	(222	11)	(223	6)
(234	6)	(235	4)	(236	38)	(237	10)	(238	4)
(249	4)	(250	4)	(263	8)	(264	5)	(265	41)
(266	24)	(267	7)	(280	12)	(281	161)	(282	30)
(283	14)	(293	3)	(294	27)	(295	5)	(296	4)
(308	6)	(309	3)	(353	12)	(354	5)	(355	16)
(356	6)	(357	3)	(383	3)	(384	22)	(385	7)
(386	3)								

NAME:13C_1623.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:162001-11-1

RI:1623

RT:9.712

NUM PEAKS: 90

(70	9)	(71	13)	(72	63)	(73	1000)	(74	759)
(75	136)	(76	14)	(84	3)	(85	16)	(86	12)
(87	23)	(88	13)	(89	37)	(90	8)	(91	3)
(99	5)	(100	15)	(101	54)	(102	80)	(103	118)
(104	24)	(105	11)	(110	3)	(113	3)	(114	6)
(115	13)	(116	15)	(117	88)	(118	26)	(119	28)
(120	3)	(129	4)	(130	26)	(131	83)	(132	59)
(133	42)	(134	10)	(135	3)	(143	3)	(144	15)
(145	37)	(146	650)	(147	215)	(148	66)	(149	17)
(150	3)	(157	4)	(158	17)	(159	16)	(160	8)
(161	11)	(162	61)	(163	13)	(164	6)	(173	10)
(174	18)	(175	14)	(176	7)	(177	4)	(189	5)
(190	9)	(191	10)	(192	6)	(203	6)	(204	3)
(205	6)	(206	42)	(207	8)	(208	3)	(218	7)
(219	14)	(220	47)	(221	15)	(222	5)	(232	4)
(233	4)	(234	4)	(235	8)	(236	8)	(246	4)
(247	4)	(248	31)	(249	25)	(263	8)	(264	11)
(265	3)	(352	3)	(353	26)	(354	8)	(355	4)

NAME:13C_1652.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:165002-11-1

RI:1652

RT:9.937

NUM PEAKS: 30

(73	1000)	(74	90)	(85	29)	(87	28)	(101	53)
(115	94)	(116	75)	(117	31)	(129	25)	(130	62)
(131	57)	(144	26)	(145	14)	(146	115)	(147	159)
(158	27)	(159	26)	(173	81)	(174	40)	(202	21)

76

(203 244) (204 48) (205 17) (217 20) (232 24)
 (319 17) (320 165) (321 41) (322 17) (335 14)

NAME:13C_1659.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:166002-11-1

RI:1659

RT:9.991

NUM PEAKS: 24

(70 15) (71 66) (72 17) (73 1000) (74 74)
 (90 26) (99 14) (103 36) (104 137) (113 15)
 (119 132) (131 28) (132 39) (133 76) (147 266)
 (148 36) (161 16) (173 36) (191 58) (203 85)
 (206 309) (207 116) (208 32) (220 52)

NAME:13C_1670.3_1313EC11_Arabinose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1670 |RI:1670 |RI:1670

CASNO:167002-11-1

RI:1670

RT:10.078

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 63

(71 18) (73 1000) (74 76) (88 12) (90 17)
 (103 60) (104 402) (105 56) (106 16) (119 44)
 (120 9) (121 7) (131 35) (132 57) (133 84)
 (134 45) (135 9) (147 227) (148 39) (149 25)
 (150 5) (161 12) (162 43) (163 19) (164 8)
 (174 7) (177 14) (190 5) (191 61) (192 25)
 (193 9) (203 10) (205 7) (206 22) (207 28)
 (208 11) (216 4) (217 16) (219 12) (220 206)
 (221 43) (222 21) (235 19) (237 5) (240 4)
 (261 7) (265 11) (275 5) (282 3) (298 4)
 (307 7) (310 73) (311 22) (312 11) (371 5)
 (440 6) (477 5) (493 4) (504 4) (522 5)
 (523 4) (568 3) (584 3)

NAME:13C_1683.3_1313EC11_Aspargine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168001-11-1

RI:1683

RT:10.179

NUM PEAKS: 90

(70 10) (71 19) (72 41) (73 1000) (74 145)
 (75 265) (76 21) (77 12) (84 5) (85 11)
 (86 10) (87 17) (88 8) (89 5) (90 7)
 (99 4) (100 18) (101 69) (102 71) (103 19)
 (115 9) (116 30) (117 54) (118 391) (119 39)
 (120 18) (128 12) (129 3) (130 12) (131 42)
 (132 47) (133 102) (134 195) (135 23) (136 7)
 (143 9) (144 119) (145 21) (146 25) (147 160)
 (148 29) (149 27) (150 4) (158 4) (159 5)
 (160 4) (161 5) (162 46) (163 7) (164 3)
 (172 3) (173 18) (174 9) (175 10) (176 4)
 (177 3) (188 4) (189 108) (190 32) (191 12)
 (192 8) (202 5) (203 3) (204 35) (205 11)
 (206 14) (207 3) (208 3) (216 4) (217 4)
 (218 20) (219 12) (220 31) (221 7) (222 3)
 (232 4) (233 10) (234 146) (235 28) (236 13)
 (246 3) (247 9) (248 4) (249 4) (262 26)
 (263 8) (264 3) (320 4) (337 7) (352 6)

NAME:13C_1713.4_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1713 |RI:1713

CASNO:171008-11-1

RI:1713

RT:10.412

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 115

(73 1000)	(74 100)	(90 38)	(92 9)	(104 419)
(105 30)	(106 13)	(107 7)	(118 17)	(119 145)
(120 11)	(132 179)	(137 6)	(165 7)	(177 13)
(180 7)	(191 48)	(192 41)	(193 8)	(194 4)
(206 48)	(207 173)	(208 35)	(209 14)	(213 8)
(220 500)	(221 137)	(222 54)	(223 11)	(224 6)
(225 9)	(227 8)	(238 7)	(240 6)	(248 35)
(249 12)	(253 4)	(265 10)	(267 7)	(270 5)
(279 17)	(280 8)	(282 6)	(283 4)	(284 4)
(286 6)	(289 9)	(294 13)	(295 8)	(296 8)
(308 8)	(309 16)	(310 68)	(311 24)	(312 15)
(313 7)	(314 7)	(316 7)	(321 9)	(322 12)
(323 57)	(324 24)	(325 10)	(326 5)	(329 7)
(330 4)	(336 5)	(339 7)	(344 4)	(346 4)
(347 5)	(349 6)	(353 7)	(355 9)	(359 7)
(377 6)	(383 8)	(388 5)	(390 5)	(391 4)
(392 7)	(393 5)	(398 8)	(399 8)	(400 5)
(402 4)	(406 4)	(407 6)	(408 5)	(410 6)
(413 7)	(416 9)	(427 4)	(431 5)	(452 6)
(454 7)	(458 6)	(459 13)	(464 4)	(466 9)
(476 4)	(479 5)	(482 3)	(488 6)	(490 4)
(493 5)	(498 8)	(502 4)	(503 6)	(508 7)
(509 4)	(524 7)	(558 7)	(567 6)	(596 3)

NAME:13C_1758.0_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176005-11-1

RI:1758

RT:10.758

NUM PEAKS: 108

(70 54)	(71 49)	(72 115)	(73 588)	(74 1000)
(75 240)	(76 25)	(77 13)	(79 10)	(80 3)
(81 3)	(83 6)	(84 12)	(85 92)	(86 33)
(87 45)	(88 46)	(89 129)	(90 23)	(91 6)
(92 3)	(93 5)	(94 3)	(95 3)	(97 4)
(98 7)	(99 31)	(100 145)	(101 43)	(102 33)
(103 14)	(104 26)	(105 7)	(106 3)	(109 3)
(111 4)	(112 4)	(113 9)	(114 7)	(115 28)
(116 25)	(117 26)	(118 29)	(119 6)	(124 3)
(125 3)	(126 3)	(127 7)	(128 33)	(129 40)
(130 13)	(131 27)	(132 58)	(133 39)	(134 7)
(135 4)	(140 3)	(141 4)	(142 3)	(143 24)
(144 23)	(145 42)	(147 55)	(148 26)	(149 12)
(150 3)	(156 5)	(157 8)	(158 10)	(159 19)
(160 12)	(161 10)	(162 22)	(163 7)	(164 3)
(169 4)	(171 4)	(172 18)	(173 35)	(174 11)
(177 71)	(178 6)	(179 5)	(187 8)	(188 38)
(189 364)	(190 40)	(191 44)	(192 14)	(193 3)
(202 5)	(203 3)	(211 6)	(215 4)	(216 3)
(217 9)	(218 4)	(219 3)	(229 8)	(230 3)
(263 10)	(264 4)	(275 4)	(285 3)	(290 3)
(291 3)	(292 8)	(307 3)		

NAME:13C_1763.8_1313EC11_Ornithine (3TMS); Arginine {BP} (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176006-11-1

RI:1764

RT:10.803

NUM PEAKS: 81

(70	11)	(71	13)	(72	84)	(73	1000)	(74	297)
(75	200)	(76	18)	(77	7)	(84	4)	(85	19)
(86	17)	(87	211)	(88	39)	(89	13)	(90	16)
(91	4)	(99	5)	(100	28)	(101	102)	(102	47)
(103	40)	(104	13)	(105	4)	(113	8)	(114	12)
(115	18)	(116	23)	(117	32)	(118	18)	(119	11)
(129	5)	(130	78)	(131	77)	(132	41)	(133	44)
(134	7)	(135	3)	(143	3)	(144	11)	(145	15)
(146	261)	(147	141)	(148	48)	(149	16)	(150	3)
(157	5)	(158	9)	(159	29)	(160	8)	(161	24)
(162	39)	(163	5)	(173	20)	(174	35)	(175	707)
(176	127)	(177	75)	(178	8)	(190	15)	(191	200)
(192	32)	(193	9)	(203	11)	(204	4)	(205	3)
(206	5)	(218	4)	(219	5)	(220	29)	(221	7)
(222	3)	(248	12)	(249	55)	(250	10)	(251	4)
(263	16)	(264	5)	(352	4)	(353	32)	(354	10)
(355	4)								

NAME:13C_1774.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177004-11-1

RI:1774

RT:10.884

NUM PEAKS: 50

(72	17)	(73	1000)	(74	81)	(75	72)	(76	10)
(86	12)	(90	6)	(100	4)	(114	5)	(115	9)
(116	8)	(119	14)	(131	33)	(132	38)	(133	51)
(144	3)	(145	9)	(146	30)	(147	249)	(148	41)
(149	31)	(150	4)	(161	6)	(164	6)	(174	23)
(178	3)	(192	29)	(205	3)	(206	14)	(219	17)
(220	481)	(221	105)	(222	43)	(223	6)	(235	45)
(236	11)	(237	4)	(248	7)	(249	6)	(250	3)
(261	3)	(262	13)	(263	4)	(295	6)	(308	13)
(309	4)	(322	4)	(455	4)	(456	12)	(457	6)

NAME:13C_1794.5_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179002-11-1

RI:1795

RT:11.041

NUM PEAKS: 162

(70	14)	(72	26)	(75	306)	(76	47)	(80	8)
(82	13)	(85	28)	(86	32)	(87	461)	(90	19)
(92	13)	(95	16)	(100	20)	(101	158)	(103	58)
(113	26)	(122	10)	(124	13)	(126	10)	(129	16)
(130	39)	(141	10)	(143	14)	(144	19)	(146	33)
(154	12)	(160	115)	(161	74)	(171	23)	(175	1000)
(176	168)	(177	62)	(178	27)	(180	10)	(181	13)
(182	16)	(187	19)	(188	16)	(191	91)	(192	23)
(196	14)	(199	9)	(212	11)	(213	15)	(214	15)
(215	10)	(224	11)	(226	8)	(232	10)	(233	18)
(239	12)	(241	7)	(244	12)	(245	12)	(247	15)
(250	15)	(256	13)	(257	14)	(258	16)	(259	12)

(260	21)	(262	21)	(266	13)	(269	10)	(272	10)
(273	7)	(274	11)	(275	10)	(276	12)	(277	19)
(288	18)	(289	7)	(290	19)	(291	7)	(296	12)
(308	13)	(309	9)	(311	10)	(312	8)	(316	11)
(317	18)	(318	23)	(322	13)	(324	11)	(332	18)
(335	14)	(337	14)	(339	10)	(340	8)	(346	9)
(349	18)	(350	81)	(351	30)	(352	15)	(357	10)
(369	11)	(370	9)	(372	13)	(373	13)	(374	13)
(379	11)	(380	12)	(383	9)	(384	15)	(385	9)
(386	22)	(390	12)	(398	8)	(404	16)	(406	8)
(407	13)	(413	9)	(414	14)	(421	14)	(423	25)
(424	20)	(426	9)	(427	17)	(433	9)	(435	8)
(438	12)	(447	9)	(453	12)	(456	13)	(463	11)
(464	13)	(466	9)	(468	9)	(470	14)	(471	12)
(476	12)	(477	21)	(478	11)	(480	12)	(481	12)
(482	14)	(483	14)	(487	10)	(490	14)	(494	8)
(496	12)	(503	19)	(510	17)	(511	12)	(513	17)
(515	11)	(517	11)	(522	15)	(524	17)	(525	9)
(530	11)	(534	13)	(537	12)	(546	9)	(547	9)
(549	9)	(555	8)	(565	11)	(567	11)	(571	12)
(577	5)	(593	4)						

NAME:13C_1809.0_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181005-11-1

RI:1809

RT:11.153

NUM PEAKS: 13

(73	1000)	(118	18)	(119	58)	(131	53)	(133	66)
(147	162)	(148	33)	(192	423)	(193	87)	(206	721)
(207	121)	(208	38)	(220	107)				

NAME:13C_1813.5_1313EC11_Glyceric acid-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181003-11-1

RI:1814

RT:11.189

NUM PEAKS: 40

(72	21)	(73	1000)	(74	81)	(75	106)	(77	14)
(103	96)	(105	12)	(117	8)	(118	29)	(119	23)
(121	8)	(131	22)	(133	111)	(134	13)	(135	35)
(147	233)	(148	40)	(149	21)	(181	18)	(191	24)
(193	20)	(195	17)	(211	130)	(212	19)	(225	18)
(227	101)	(228	15)	(255	8)	(285	15)	(299	137)
(300	35)	(315	47)	(316	14)	(358	12)	(359	68)
(360	18)	(361	8)	(387	32)	(388	14)	(462	15)

NAME:13C_1852.0_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185004-11-1

RI:1852

RT:11.487

NUM PEAKS: 33

(75	1000)	(76	100)	(77	67)	(81	48)	(118	188)
(119	463)	(129	239)	(131	85)	(132	469)	(134	270)
(135	49)	(143	33)	(145	114)	(150	20)	(153	19)
(163	32)	(192	29)	(205	47)	(208	25)	(213	22)
(239	12)	(286	49)	(299	109)	(312	19)	(334	18)
(379	20)	(380	13)	(382	16)	(412	17)	(413	17)
(441	22)	(462	12)	(483	17)				

NAME:13C_1878.9_1313EC11_alpha-D-Methylglucopyranoside (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188006-11-1

RI:1879

RT:11.695

NUM PEAKS: 45

(73 1000)	(74 100)	(76 41)	(77 11)	(93 16)
(96 2)	(97 2)	(100 6)	(113 3)	(118 35)
(121 13)	(122 5)	(123 3)	(127 2)	(134 235)
(135 26)	(136 8)	(150 39)	(151 4)	(167 13)
(168 3)	(169 3)	(171 2)	(174 17)	(179 2)
(189 9)	(196 2)	(197 6)	(205 20)	(206 500)
(223 22)	(224 3)	(245 9)	(246 2)	(247 2)
(250 3)	(268 7)	(269 33)	(270 6)	(271 2)
(277 4)	(284 5)	(293 10)	(351 2)	(383 4)

NAME:13C_1882.2_1313EC11_Mannose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188002-11-1

RI:1882

RT:11.721

NUM PEAKS: 62

(70 6)	(72 18)	(73 1000)	(74 84)	(75 136)
(87 37)	(88 20)	(90 13)	(101 29)	(102 16)
(105 27)	(114 3)	(115 24)	(117 18)	(119 78)
(120 5)	(130 15)	(131 75)	(132 112)	(133 43)
(144 8)	(145 11)	(147 343)	(148 37)	(160 70)
(161 116)	(162 170)	(163 26)	(164 7)	(178 6)
(203 10)	(207 173)	(208 20)	(209 13)	(210 3)
(211 7)	(216 4)	(219 13)	(232 5)	(233 29)
(234 49)	(235 14)	(236 7)	(251 3)	(260 3)
(278 6)	(294 22)	(295 5)	(296 5)	(299 11)
(308 3)	(321 4)	(322 31)	(323 167)	(324 51)
(325 20)	(341 4)	(359 8)	(370 4)	(373 5)
(469 3)	(514 4)			

NAME:13C_1888.8_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189005-11-1

RI:1889

RT:11.772

NUM PEAKS: 5

(192 571)	(193 87)	(194 40)	(206 1000)	(441 7)
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NAME:13C_1893.5_1313EC11_Glucose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189002-11-1

RI:1894

RT:11.808

NUM PEAKS: 91

(70 6)	(71 6)	(72 17)	(73 1000)	(74 98)
(75 91)	(76 4)	(85 5)	(86 10)	(87 33)
(88 6)	(89 45)	(90 33)	(91 5)	(100 3)
(101 22)	(102 16)	(103 42)	(104 131)	(105 53)
(106 10)	(114 4)	(115 11)	(116 24)	(117 15)
(118 14)	(119 126)	(120 11)	(121 5)	(129 4)
(130 10)	(131 46)	(132 186)	(133 106)	(134 39)
(135 10)	(144 4)	(145 12)	(146 24)	(147 486)
(148 82)	(149 48)	(150 6)	(159 4)	(160 9)

81

(161	126)	(162	232)	(163	49)	(164	17)	(173	6)
(174	6)	(175	4)	(176	7)	(177	9)	(178	6)
(189	4)	(190	7)	(191	52)	(193	7)	(203	6)
(204	5)	(205	6)	(207	240)	(208	47)	(209	22)
(218	5)	(219	18)	(220	131)	(221	38)	(222	15)
(223	3)	(232	3)	(233	39)	(234	19)	(235	23)
(236	8)	(237	3)	(247	3)	(248	7)	(249	6)
(250	4)	(261	3)	(264	3)	(275	4)	(306	3)
(308	6)	(310	5)	(322	14)	(323	188)	(368	5)
(380	3)								

NAME:13C_1914.8_1313EC11_Glucose methoxyamine {BP} (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:191001-11-1

RI:1915

RT:11.953

NUM PEAKS: 68

(73	1000)	(75	54)	(87	18)	(89	67)	(90	29)
(91	5)	(101	17)	(103	31)	(104	208)	(105	37)
(106	10)	(118	11)	(119	92)	(120	10)	(121	4)
(132	126)	(133	76)	(134	38)	(135	9)	(145	5)
(147	332)	(148	54)	(149	35)	(150	4)	(161	85)
(162	133)	(163	31)	(164	10)	(173	4)	(177	8)
(178	6)	(190	6)	(191	36)	(192	16)	(193	5)
(203	3)	(204	3)	(205	5)	(206	40)	(207	188)
(208	36)	(209	16)	(219	8)	(220	86)	(221	24)
(222	10)	(233	26)	(234	8)	(235	22)	(236	7)
(237	9)	(248	5)	(249	4)	(250	3)	(274	3)
(278	5)	(279	8)	(280	3)	(294	10)	(295	3)
(308	5)	(309	3)	(310	5)	(322	12)	(323	159)
(324	46)	(325	23)	(326	4)				

NAME:13C_1931.9_1313EC11_Sorbitol (6TMS); Glucitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193001-11-1

RI:1932

RT:12.062

NUM PEAKS: 79

(71	4)	(72	20)	(73	1000)	(74	85)	(75	68)
(76	4)	(87	17)	(88	5)	(89	9)	(90	28)
(91	3)	(102	11)	(103	33)	(104	179)	(105	19)
(106	7)	(115	5)	(116	5)	(117	7)	(118	10)
(119	107)	(120	8)	(121	4)	(131	27)	(132	92)
(133	73)	(134	12)	(135	6)	(145	4)	(146	14)
(147	344)	(148	59)	(149	35)	(150	4)	(160	8)
(161	73)	(162	7)	(163	5)	(164	4)	(177	7)
(178	3)	(189	10)	(191	39)	(192	35)	(193	9)
(205	6)	(206	50)	(207	157)	(208	29)	(209	12)
(219	6)	(220	165)	(221	40)	(222	16)	(223	3)
(233	16)	(234	7)	(235	17)	(236	3)	(261	7)
(264	5)	(279	8)	(280	4)	(294	8)	(308	6)
(309	8)	(310	26)	(311	7)	(312	3)	(322	12)
(323	127)	(324	36)	(325	17)	(326	3)	(336	10)
(337	3)	(351	6)	(425	3)	(426	4)		

NAME:13C_1956.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:196004-11-1

RI:1956

RT:12.216

82

NUM PEAKS: 94

(70	4)	(72	20)	(73	1000)	(74	92)	(75	122)
(76	9)	(77	9)	(86	29)	(87	12)	(88	6)
(89	35)	(90	26)	(91	7)	(100	3)	(101	12)
(102	13)	(103	32)	(104	99)	(105	21)	(106	5)
(114	6)	(115	17)	(116	9)	(117	11)	(118	14)
(119	59)	(120	6)	(129	4)	(130	7)	(131	28)
(132	116)	(133	74)	(134	18)	(135	8)	(144	8)
(145	12)	(146	19)	(147	174)	(148	36)	(149	46)
(150	5)	(151	3)	(158	5)	(159	5)	(160	15)
(162	18)	(163	21)	(164	4)	(173	7)	(174	57)
(175	32)	(176	12)	(177	12)	(178	4)	(190	10)
(191	36)	(192	24)	(193	6)	(203	3)	(204	3)
(205	6)	(206	57)	(207	21)	(208	7)	(218	4)
(219	12)	(220	226)	(221	43)	(222	30)	(223	5)
(232	3)	(233	6)	(234	6)	(235	6)	(246	3)
(247	7)	(248	32)	(249	12)	(250	5)	(251	5)
(264	5)	(265	3)	(277	17)	(278	4)	(294	4)
(308	4)	(323	7)	(336	6)	(337	13)	(338	5)
(366	7)	(367	41)	(368	13)	(369	6)		

NAME:13C_1973.5_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:197002-11-1

RI:1974

RT:12.326

NUM PEAKS: 61

(70	4)	(72	19)	(73	1000)	(74	86)	(75	97)
(77	3)	(86	9)	(87	9)	(88	4)	(90	13)
(101	5)	(102	8)	(103	34)	(104	59)	(105	9)
(106	3)	(114	3)	(115	8)	(117	8)	(118	17)
(119	36)	(120	3)	(131	27)	(132	67)	(133	67)
(134	11)	(135	6)	(145	4)	(146	17)	(147	227)
(148	37)	(160	7)	(161	11)	(164	3)	(176	3)
(177	4)	(178	3)	(189	3)	(191	47)	(192	270)
(193	47)	(194	20)	(204	8)	(205	13)	(206	441)
(207	81)	(208	36)	(209	4)	(220	84)	(221	28)
(222	11)	(234	3)	(235	9)	(236	4)	(248	6)
(294	6)	(308	6)	(322	3)	(323	4)	(351	3)
(441	3)								

NAME:13C_1999.9_1313EC11_Gluconic acid (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200001-11-1

RI:2000

RT:12.494

NUM PEAKS: 62

(73	1000)	(81	19)	(82	28)	(90	16)	(96	19)
(98	15)	(103	22)	(104	95)	(105	13)	(109	5)
(112	12)	(119	66)	(124	6)	(125	22)	(127	4)
(132	63)	(133	65)	(134	11)	(135	8)	(147	349)
(148	57)	(149	38)	(161	26)	(168	5)	(191	39)
(192	23)	(206	40)	(207	68)	(208	13)	(209	7)
(220	87)	(221	28)	(222	17)	(233	7)	(248	9)
(249	7)	(261	4)	(266	4)	(279	14)	(294	67)
(295	23)	(296	11)	(308	29)	(309	13)	(310	11)
(311	5)	(323	29)	(336	18)	(337	64)	(338	23)
(339	12)	(340	6)	(344	5)	(346	6)	(350	5)
(364	8)	(365	14)	(428	5)	(454	4)	(505	7)
(528	4)	(550	4)						

NAME:13C_2026.0_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:203003-11-1

RI:2026

RT:12.660

NUM PEAKS: 53

(71	4)	(73	1000)	(74	74)	(86	6)	(89	41)
(90	15)	(91	6)	(101	39)	(103	29)	(104	46)
(105	13)	(131	20)	(133	51)	(145	4)	(146	12)
(147	175)	(148	18)	(149	45)	(150	4)	(160	4)
(161	27)	(162	5)	(164	3)	(173	7)	(174	14)
(175	4)	(176	3)	(189	3)	(191	29)	(192	20)
(193	5)	(205	8)	(206	325)	(207	73)	(208	28)
(209	4)	(219	5)	(220	74)	(221	83)	(222	20)
(223	7)	(233	6)	(234	4)	(235	15)	(236	4)
(249	4)	(264	6)	(294	3)	(308	4)	(322	6)
(323	56)	(324	16)	(325	7)				

NAME:13C_2028.6_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:203002-11-1

RI:2029

RT:12.676

NUM PEAKS: 88

(70	33)	(71	34)	(72	236)	(74	190)	(75	1000)
(76	82)	(77	52)	(82	3)	(83	29)	(84	19)
(85	101)	(86	45)	(87	185)	(88	114)	(89	168)
(93	3)	(96	3)	(97	5)	(98	35)	(99	12)
(100	60)	(102	213)	(103	102)	(104	101)	(106	14)
(113	15)	(114	6)	(115	32)	(116	38)	(117	77)
(118	146)	(119	527)	(120	42)	(121	20)	(126	3)
(127	4)	(128	22)	(129	9)	(130	32)	(131	42)
(132	468)	(134	188)	(135	31)	(136	8)	(137	3)
(141	3)	(142	4)	(143	19)	(144	20)	(145	18)
(146	35)	(148	164)	(150	10)	(157	3)	(158	12)
(159	10)	(160	23)	(162	39)	(163	47)	(164	5)
(165	5)	(175	15)	(176	21)	(177	28)	(178	16)
(179	4)	(181	3)	(188	3)	(189	6)	(190	16)
(193	8)	(194	4)	(204	3)	(237	6)	(238	6)
(239	3)	(250	3)	(251	5)	(252	29)	(253	5)
(254	4)	(301	3)	(326	22)	(327	106)	(328	15)
(329	4)	(341	3)	(342	10)				

NAME:13C_2039.3_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:204003-11-1

RI:2039

RT:12.745

NUM PEAKS: 56

(73	1000)	(74	83)	(87	116)	(101	75)	(102	49)
(115	34)	(130	113)	(131	46)	(133	47)	(145	24)
(147	143)	(149	20)	(152	14)	(159	23)	(171	9)
(173	37)	(175	313)	(176	58)	(177	53)	(183	15)
(189	18)	(190	18)	(195	9)	(203	57)	(216	18)
(217	33)	(218	346)	(219	65)	(222	10)	(231	18)
(242	16)	(262	16)	(275	16)	(277	17)	(292	41)
(293	21)	(345	15)	(346	7)	(378	17)	(379	39)
(396	16)	(425	12)	(432	11)	(438	8)	(449	12)
(453	15)	(462	14)	(463	17)	(473	16)	(476	13)

84

(491 15) (508 17) (557 9) (566 14) (571 8)
 (585 4)

NAME:13C_2048.0_1313EC11_Hexadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:205001-11-1

RI:2048

RT:12.800

NUM PEAKS: 86

(70 8) (72 95) (73 1000) (74 227) (75 996)
 (76 109) (77 53) (85 23) (86 10) (87 82)
 (88 37) (89 108) (90 12) (91 15) (100 22)
 (101 12) (102 76) (103 42) (104 65) (105 6)
 (106 28) (107 3) (115 9) (118 161) (119 904)
 (120 71) (121 35) (130 13) (132 489) (133 68)
 (134 607) (135 85) (136 26) (137 3) (140 4)
 (147 53) (148 223) (149 34) (150 11) (160 7)
 (161 6) (162 16) (163 28) (164 11) (175 4)
 (177 22) (178 9) (179 6) (192 32) (193 24)
 (194 8) (206 4) (207 14) (208 50) (209 7)
 (210 3) (211 3) (220 3) (222 10) (223 8)
 (224 3) (233 3) (237 8) (238 11) (239 3)
 (252 5) (253 11) (267 3) (268 6) (282 7)
 (283 3) (284 6) (297 4) (298 12) (299 11)
 (300 3) (315 4) (327 10) (328 38) (329 194)
 (330 28) (331 7) (343 6) (344 21) (345 3)
 (387 4)

NAME:13C_2087.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209004-11-1

RI:2087

RT:13.049

NUM PEAKS: 65

(71 8) (72 21) (73 1000) (74 86) (75 87)
 (76 7) (85 9) (86 14) (87 10) (89 71)
 (90 23) (91 7) (101 45) (102 15) (103 31)
 (104 65) (105 16) (106 4) (114 5) (116 6)
 (117 13) (118 16) (119 42) (131 23) (132 74)
 (133 49) (134 12) (145 8) (146 17) (147 157)
 (148 32) (149 50) (150 7) (160 8) (161 32)
 (162 10) (163 9) (164 5) (173 10) (174 12)
 (176 6) (187 3) (192 19) (193 4) (202 3)
 (205 7) (206 362) (207 84) (208 30) (209 5)
 (220 75) (221 92) (222 22) (223 7) (233 9)
 (234 6) (235 18) (248 11) (249 4) (264 5)
 (294 7) (322 9) (323 69) (324 20) (325 9)

NAME:13C_2063.4_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:206001-11-1

RI:2063

RT:12.898

NUM PEAKS: 296

(70 45) (71 26) (72 65) (74 180) (75 213)
 (79 27) (80 24) (81 33) (86 33) (87 255)
 (89 32) (91 29) (95 34) (99 33) (100 24)
 (101 131) (103 110) (105 33) (106 48) (109 37)
 (112 26) (113 32) (114 36) (115 62) (116 33)
 (117 99) (118 52) (119 205) (120 42) (122 42)

(125	21)	(126	20)	(128	33)	(130	37)	(131	72)
(132	33)	(133	116)	(135	31)	(137	25)	(139	26)
(140	51)	(141	19)	(142	25)	(143	28)	(144	40)
(145	42)	(147	308)	(148	107)	(149	59)	(150	23)
(151	45)	(153	31)	(157	31)	(159	31)	(160	60)
(161	48)	(164	31)	(165	42)	(166	22)	(167	21)
(168	24)	(169	27)	(171	23)	(173	40)	(174	56)
(175	1000)	(176	223)	(177	161)	(178	42)	(179	52)
(180	22)	(182	29)	(186	22)	(188	25)	(189	66)
(192	47)	(201	49)	(205	39)	(206	23)	(208	19)
(209	26)	(210	22)	(211	69)	(212	60)	(213	35)
(214	24)	(215	39)	(217	29)	(219	31)	(221	32)
(222	27)	(224	41)	(225	26)	(226	30)	(227	41)
(230	29)	(231	37)	(232	23)	(233	28)	(234	26)
(235	37)	(236	47)	(237	33)	(239	21)	(243	22)
(246	33)	(247	59)	(248	91)	(249	29)	(254	33)
(255	33)	(256	33)	(257	36)	(261	20)	(262	42)
(263	130)	(264	46)	(265	38)	(266	41)	(268	30)
(269	27)	(271	26)	(273	18)	(274	43)	(275	37)
(276	29)	(277	20)	(278	31)	(279	37)	(281	44)
(282	25)	(289	22)	(291	20)	(292	36)	(295	22)
(297	28)	(299	63)	(303	24)	(305	34)	(310	29)
(312	24)	(313	42)	(314	24)	(315	61)	(318	40)
(321	30)	(322	21)	(323	27)	(324	48)	(325	43)
(328	36)	(329	35)	(330	38)	(332	30)	(334	39)
(335	17)	(337	38)	(338	44)	(340	26)	(341	34)
(344	22)	(346	18)	(347	31)	(350	23)	(355	29)
(356	49)	(357	27)	(359	24)	(360	24)	(361	29)
(364	25)	(365	29)	(371	30)	(374	38)	(376	32)
(377	20)	(383	20)	(384	50)	(385	50)	(386	29)
(387	21)	(388	28)	(389	33)	(390	29)	(394	25)
(395	33)	(397	35)	(398	25)	(399	29)	(401	21)
(404	22)	(405	26)	(406	40)	(407	31)	(408	31)
(409	19)	(411	24)	(412	25)	(414	32)	(417	21)
(418	36)	(419	22)	(420	23)	(422	31)	(423	34)
(424	27)	(425	26)	(426	29)	(427	29)	(428	21)
(431	26)	(432	23)	(433	24)	(434	32)	(435	22)
(437	23)	(438	30)	(441	22)	(442	29)	(446	34)
(448	33)	(449	16)	(451	20)	(453	31)	(454	49)
(455	98)	(456	50)	(457	41)	(459	21)	(460	25)
(461	39)	(462	37)	(465	29)	(466	25)	(467	47)
(468	25)	(469	27)	(472	34)	(473	37)	(477	22)
(480	25)	(481	25)	(482	38)	(483	30)	(485	27)
(487	27)	(488	35)	(492	30)	(493	35)	(494	28)
(495	34)	(496	30)	(498	26)	(499	42)	(500	25)
(501	44)	(503	22)	(504	36)	(508	30)	(509	26)
(510	36)	(514	30)	(515	23)	(516	23)	(517	35)
(518	32)	(519	30)	(521	22)	(522	29)	(523	22)
(524	29)	(526	25)	(527	22)	(528	37)	(529	33)
(531	26)	(533	34)	(535	56)	(536	45)	(537	36)
(538	26)	(539	19)	(542	30)	(546	35)	(547	52)
(550	24)	(554	25)	(560	18)	(564	30)	(565	15)
(566	21)	(570	23)	(571	21)	(579	22)	(583	14)
(592	14)								

NAME:13C_2025.7_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203004-11-1

RI:2026

RT:12.686

NUM PEAKS: 343

(70	22)	(71	55)	(72	44)	(73	1000)	(74	58)
(75	317)	(76	5)	(77	20)	(78	11)	(79	11)
(80	8)	(81	8)	(82	4)	(83	17)	(84	38)
(85	50)	(86	29)	(87	24)	(88	17)	(90	7)
(92	9)	(93	6)	(94	3)	(96	5)	(97	7)
(98	11)	(99	20)	(100	35)	(101	5)	(102	41)
(103	40)	(104	11)	(105	18)	(106	9)	(107	21)
(109	4)	(111	4)	(112	9)	(113	3)	(114	14)
(115	35)	(116	27)	(117	10)	(118	17)	(119	38)
(122	12)	(123	15)	(127	11)	(129	10)	(130	8)
(131	59)	(132	79)	(133	96)	(135	18)	(137	22)
(138	4)	(141	9)	(142	3)	(143	10)	(144	5)
(145	11)	(146	20)	(147	194)	(148	46)	(149	13)
(150	4)	(151	9)	(153	16)	(154	6)	(155	15)
(156	17)	(157	8)	(162	18)	(164	4)	(165	12)
(167	18)	(169	5)	(170	4)	(171	3)	(172	14)
(173	22)	(174	155)	(175	31)	(176	12)	(177	6)
(178	7)	(179	3)	(181	16)	(182	4)	(183	20)
(185	4)	(187	7)	(188	15)	(189	43)	(190	8)
(191	5)	(192	3)	(193	20)	(194	7)	(195	7)
(196	7)	(197	10)	(199	3)	(200	10)	(202	5)
(203	9)	(204	3)	(205	6)	(210	10)	(211	106)
(212	23)	(213	3)	(214	10)	(215	3)	(216	15)
(217	5)	(218	15)	(219	13)	(223	4)	(224	8)
(225	16)	(226	9)	(227	35)	(228	13)	(229	8)
(230	5)	(231	3)	(233	7)	(234	6)	(240	4)
(241	15)	(242	4)	(243	24)	(244	6)	(245	7)
(246	4)	(247	69)	(248	190)	(249	54)	(250	11)
(251	10)	(252	8)	(253	6)	(254	9)	(255	10)
(256	10)	(257	8)	(259	4)	(260	3)	(261	5)
(262	27)	(263	134)	(264	34)	(265	8)	(266	3)
(267	10)	(268	6)	(269	6)	(273	4)	(276	7)
(277	5)	(278	11)	(279	18)	(280	5)	(282	13)
(283	8)	(284	8)	(285	4)	(289	3)	(290	12)
(291	8)	(292	5)	(293	7)	(294	5)	(295	3)
(296	6)	(297	5)	(298	14)	(299	122)	(300	56)
(301	19)	(302	7)	(303	9)	(304	3)	(307	6)
(308	5)	(309	6)	(313	13)	(314	14)	(315	101)
(316	29)	(317	13)	(320	3)	(325	16)	(326	19)
(327	21)	(330	3)	(332	3)	(333	5)	(334	9)
(335	3)	(336	11)	(337	9)	(338	6)	(341	12)
(342	16)	(345	3)	(346	13)	(347	8)	(348	6)
(349	11)	(350	7)	(352	9)	(353	6)	(354	3)
(355	6)	(356	10)	(357	8)	(360	4)	(361	14)
(362	7)	(363	3)	(364	18)	(365	12)	(366	3)
(368	4)	(369	8)	(371	9)	(372	5)	(373	3)
(374	3)	(376	4)	(382	3)	(383	3)	(388	3)
(389	10)	(391	3)	(398	6)	(399	6)	(401	9)
(402	6)	(403	5)	(404	4)	(405	3)	(407	4)
(408	5)	(409	4)	(410	9)	(411	15)	(412	6)
(414	5)	(415	10)	(420	8)	(421	11)	(422	3)
(423	3)	(427	6)	(428	7)	(430	7)	(431	13)
(432	10)	(433	9)	(434	3)	(436	6)	(441	7)
(444	5)	(445	3)	(446	7)	(452	7)	(453	6)
(454	3)	(455	7)	(456	6)	(457	10)	(458	9)
(461	8)	(462	14)	(468	4)	(469	11)	(471	8)
(472	3)	(473	7)	(477	3)	(478	11)	(480	4)
(483	4)	(484	6)	(487	4)	(488	5)	(489	7)
(490	9)	(491	8)	(492	6)	(494	7)	(497	14)

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(501	10)	(502	10)	(504	4)	(506	8)	(507	5)
(508	11)	(509	3)	(510	3)	(512	5)	(513	4)
(514	4)	(515	4)	(519	8)	(520	7)	(522	5)
(527	6)	(530	6)	(532	7)	(533	13)	(535	5)
(537	4)	(538	4)	(539	3)	(543	9)	(544	8)
(545	4)	(547	5)	(550	5)	(551	4)	(552	7)
(553	3)	(557	5)	(558	7)	(559	5)	(560	6)
(566	4)	(567	3)	(568	5)	(569	5)	(571	10)
(572	5)	(573	4)	(574	3)	(575	4)	(580	6)
(581	5)	(582	5)	(597	3)				

NAME:13C_2003.6_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200002-11-1

RI:2004

RT:12.518

NUM PEAKS: 114

(72	48)	(73	434)	(74	140)	(75	206)	(76	23)
(77	11)	(86	16)	(87	216)	(88	32)	(89	13)
(94	5)	(99	11)	(100	68)	(101	111)	(102	42)
(103	22)	(113	10)	(114	7)	(115	34)	(116	31)
(117	50)	(118	51)	(123	5)	(129	15)	(130	72)
(131	114)	(134	7)	(135	7)	(137	5)	(143	27)
(144	16)	(145	12)	(146	126)	(150	6)	(152	4)
(156	9)	(157	13)	(158	7)	(159	27)	(160	50)
(163	4)	(169	5)	(173	28)	(174	22)	(175	1000)
(176	169)	(177	78)	(178	6)	(184	4)	(188	6)
(189	13)	(190	15)	(199	5)	(200	20)	(203	12)
(204	8)	(205	44)	(211	5)	(215	11)	(216	7)
(218	14)	(219	7)	(221	15)	(230	10)	(231	102)
(232	19)	(233	6)	(234	11)	(235	10)	(245	5)
(250	6)	(259	6)	(264	10)	(265	21)	(266	5)
(283	4)	(284	6)	(287	4)	(288	5)	(289	5)
(290	5)	(291	9)	(292	9)	(297	6)	(299	7)
(306	6)	(316	7)	(317	6)	(320	6)	(321	20)
(324	24)	(325	6)	(334	6)	(335	5)	(369	4)
(370	6)	(380	4)	(381	5)	(382	18)	(383	6)
(389	5)	(396	5)	(397	9)	(418	5)	(424	5)
(436	6)	(443	4)	(452	5)	(456	5)	(481	5)
(495	5)	(534	6)	(544	4)	(548	5)		

NAME:13C_1878.0_1313EC11_Fructose methoxyamine {BP} (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188004-11-1

RI:1878

RT:11.688

NUM PEAKS: 68

(70	5)	(71	7)	(72	20)	(73	1000)	(74	92)
(75	79)	(85	24)	(86	13)	(88	6)	(89	55)
(90	27)	(91	4)	(101	9)	(102	9)	(103	50)
(104	222)	(105	34)	(106	9)	(114	3)	(115	7)
(116	21)	(117	10)	(118	19)	(119	59)	(120	8)
(129	3)	(130	3)	(131	24)	(132	70)	(133	76)
(135	12)	(145	8)	(146	14)	(147	217)	(148	52)
(164	3)	(175	3)	(176	11)	(177	8)	(178	3)
(190	4)	(191	32)	(192	24)	(193	6)	(203	7)
(204	6)	(208	17)	(219	11)	(220	172)	(221	40)
(222	18)	(235	7)	(236	3)	(248	6)	(249	3)
(262	4)	(265	8)	(266	5)	(279	10)	(280	4)
(294	3)	(308	3)	(309	5)	(310	40)	(311	11)

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(312 5) (338 4) (368 6)

NAME:13C_1824.4_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182006-11-1

RI:1824

RT:11.274

NUM PEAKS: 205

(76 309)	(77 511)	(78 165)	(79 428)	(81 43)
(82 42)	(83 61)	(84 208)	(91 135)	(92 44)
(93 247)	(94 42)	(95 133)	(96 59)	(97 112)
(107 30)	(108 23)	(109 22)	(110 35)	(111 51)
(112 42)	(120 31)	(121 32)	(124 13)	(125 41)
(126 58)	(127 78)	(137 24)	(140 38)	(141 87)
(142 52)	(152 37)	(153 27)	(154 25)	(155 57)
(156 34)	(165 30)	(169 62)	(170 124)	(182 23)
(184 117)	(195 28)	(196 48)	(197 73)	(198 118)
(199 35)	(200 20)	(210 49)	(212 106)	(214 31)
(224 27)	(225 25)	(226 26)	(227 27)	(228 29)
(240 27)	(241 33)	(242 49)	(243 36)	(244 22)
(245 43)	(254 35)	(255 23)	(256 26)	(268 25)
(269 204)	(270 1000)	(271 209)	(272 97)	(282 21)
(283 27)	(284 98)	(285 353)	(286 82)	(287 34)
(288 10)	(296 10)	(297 8)	(298 19)	(299 75)
(300 19)	(302 22)	(304 25)	(310 60)	(311 38)
(312 26)	(313 22)	(314 32)	(315 30)	(316 19)
(317 16)	(324 24)	(325 30)	(326 14)	(327 21)
(328 27)	(329 12)	(330 21)	(331 26)	(332 19)
(333 35)	(340 10)	(341 9)	(342 12)	(345 15)
(346 23)	(356 10)	(359 9)	(362 24)	(366 29)
(371 13)	(372 11)	(378 12)	(387 18)	(388 7)
(391 10)	(394 13)	(395 14)	(396 15)	(397 21)
(398 25)	(399 16)	(400 17)	(401 15)	(404 20)
(405 20)	(406 10)	(414 17)	(415 19)	(416 15)
(417 16)	(418 18)	(419 17)	(420 23)	(421 15)
(422 22)	(430 11)	(431 14)	(432 12)	(434 14)
(435 12)	(436 10)	(437 13)	(438 24)	(439 18)
(440 19)	(441 9)	(442 13)	(443 18)	(444 21)
(445 9)	(452 10)	(453 10)	(454 11)	(456 12)
(464 26)	(466 28)	(467 17)	(468 11)	(469 16)
(474 20)	(475 13)	(489 9)	(492 12)	(493 14)
(494 14)	(495 17)	(496 8)	(497 13)	(501 12)
(505 8)	(506 8)	(509 12)	(511 18)	(512 21)
(513 17)	(514 13)	(516 16)	(517 13)	(518 19)
(520 12)	(521 9)	(522 23)	(523 12)	(524 13)
(525 12)	(526 20)	(527 17)	(528 19)	(529 9)
(530 11)	(531 14)	(536 8)	(538 11)	(540 10)
(541 18)	(542 14)	(543 8)	(546 13)	(548 15)
(552 7)	(556 4)	(561 8)	(588 4)	(592 4)

NAME:13C_1822.9_1313EC11_Citric acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182004-11-1

RI:1823

RT:11.261

NUM PEAKS: 145

(70 24)	(71 111)	(72 59)	(73 1000)	(74 10)
(75 352)	(76 22)	(77 29)	(78 3)	(79 5)
(83 4)	(84 9)	(85 24)	(89 4)	(93 12)
(95 8)	(96 5)	(97 9)	(98 5)	(99 21)

(100	8)	(105	8)	(111	5)	(118	13)	(119	10)
(127	3)	(129	10)	(132	8)	(133	110)	(134	10)
(135	12)	(139	4)	(141	9)	(142	3)	(143	15)
(147	526)	(148	33)	(149	126)	(150	16)	(151	10)
(155	3)	(161	4)	(163	13)	(169	5)	(170	5)
(171	4)	(183	28)	(184	8)	(185	11)	(187	5)
(188	75)	(189	16)	(190	9)	(191	6)	(193	4)
(197	3)	(198	4)	(201	3)	(207	19)	(208	4)
(209	3)	(211	41)	(212	9)	(213	7)	(215	8)
(216	10)	(217	112)	(219	10)	(221	63)	(222	12)
(223	8)	(229	5)	(231	7)	(232	4)	(233	12)
(234	10)	(235	13)	(245	3)	(257	18)	(258	4)
(259	4)	(261	11)	(262	51)	(269	8)	(270	43)
(271	8)	(272	7)	(273	136)	(274	31)	(275	14)
(276	7)	(277	33)	(278	378)	(279	68)	(280	32)
(281	4)	(284	4)	(285	19)	(286	4)	(287	3)
(291	13)	(292	3)	(293	6)	(299	3)	(301	3)
(303	4)	(305	9)	(306	5)	(307	16)	(308	23)
(309	9)	(310	5)	(323	5)	(337	3)	(338	3)
(346	3)	(347	26)	(348	9)	(349	5)	(350	3)
(351	15)	(352	80)	(353	23)	(354	11)	(363	18)
(364	6)	(365	3)	(367	9)	(368	55)	(369	16)
(370	7)	(374	3)	(375	20)	(376	6)	(377	3)
(380	11)	(381	56)	(382	17)	(383	9)	(465	8)
(466	3)	(470	7)	(471	24)	(472	10)	(473	3)

NAME:13C_1741.3_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174003-11-1

RI:1741

RT:10.629

NUM PEAKS: 33

(72	33)	(73	1000)	(74	59)	(75	97)	(76	13)
(101	106)	(108	11)	(113	16)	(116	14)	(117	22)
(129	19)	(130	21)	(131	44)	(133	48)	(143	17)
(147	280)	(148	42)	(149	22)	(163	99)	(173	82)
(174	20)	(184	10)	(204	48)	(205	44)	(207	215)
(208	29)	(221	14)	(231	48)	(281	17)	(291	9)
(292	21)	(307	29)	(410	12)				

NAME:13C_1694.3_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:169001-11-1

RI:1694

RT:10.264

NUM PEAKS: 44

(70	12)	(73	1000)	(74	53)	(75	61)	(90	60)
(93	10)	(103	86)	(104	53)	(107	14)	(114	14)
(117	46)	(119	183)	(131	23)	(132	55)	(133	91)
(134	11)	(135	16)	(147	207)	(148	37)	(149	26)
(153	8)	(155	11)	(158	12)	(191	20)	(219	46)
(220	22)	(235	41)	(236	19)	(245	8)	(249	9)
(250	39)	(254	16)	(264	29)	(271	16)	(292	16)
(313	9)	(323	16)	(346	21)	(347	13)	(358	13)
(392	15)	(405	14)	(458	12)	(459	10)		

NAME:13C_1673.0_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167003-11-1

RI:1673

RT:10.101

NUM PEAKS: 60

(73 1000)	(74 100)	(75 212)	(76 15)	(85 14)
(86 50)	(87 123)	(98 3)	(99 8)	(100 11)
(102 55)	(103 476)	(112 4)	(115 29)	(117 17)
(118 27)	(127 3)	(142 3)	(144 7)	(158 11)
(159 7)	(160 39)	(161 26)	(172 3)	(175 51)
(176 28)	(184 2)	(186 3)	(187 2)	(188 4)
(189 18)	(200 2)	(201 2)	(204 5)	(214 2)
(215 2)	(229 2)	(230 2)	(248 11)	(249 9)
(250 5)	(277 3)	(292 6)	(293 69)	(294 500)
(295 99)	(296 43)	(297 5)	(321 2)	(322 8)
(323 3)	(350 2)	(351 10)	(352 4)	(353 3)
(368 13)	(369 5)	(370 2)	(396 2)	(397 2)

NAME:13C_1562.0_1313EC11_Cysteine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:156002-11-1

RI:1562

RT:9.232

NUM PEAKS: 115

(70 174)	(71 121)	(72 45)	(73 1000)	(74 199)
(75 502)	(76 45)	(77 24)	(80 9)	(81 9)
(82 17)	(83 124)	(85 100)	(86 14)	(87 44)
(88 37)	(89 41)	(90 9)	(91 49)	(92 8)
(94 5)	(95 5)	(96 35)	(97 41)	(98 351)
(99 49)	(100 68)	(101 60)	(102 39)	(103 30)
(104 55)	(105 4)	(106 6)	(110 24)	(111 140)
(112 13)	(113 17)	(114 9)	(115 13)	(116 8)
(117 23)	(118 35)	(119 31)	(120 6)	(121 4)
(123 3)	(124 6)	(125 23)	(126 63)	(127 144)
(130 5)	(131 23)	(132 250)	(133 72)	(134 26)
(135 5)	(137 3)	(139 26)	(140 8)	(141 9)
(143 12)	(145 6)	(146 5)	(147 130)	(153 5)
(154 5)	(155 9)	(156 13)	(157 6)	(158 6)
(159 67)	(161 12)	(163 8)	(168 9)	(169 10)
(172 6)	(173 9)	(174 4)	(175 14)	(177 5)
(183 6)	(184 15)	(185 21)	(187 4)	(200 3)
(201 4)	(202 18)	(206 8)	(208 4)	(212 4)
(213 42)	(214 8)	(218 5)	(219 5)	(220 76)
(221 19)	(222 81)	(223 13)	(224 10)	(230 5)
(231 30)	(232 4)	(235 5)	(236 3)	(237 8)
(244 4)	(250 3)	(251 9)	(252 4)	(264 4)
(265 3)	(279 3)	(285 5)	(286 3)	(296 4)

NAME:13C_1279.2_1313EC16_Serine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:128001-11-1

RI:1279

RT:6.160

NUM PEAKS: 40

(72 20)	(73 1000)	(74 114)	(75 320)	(76 27)
(77 9)	(81 44)	(86 7)	(87 86)	(88 32)
(89 41)	(90 9)	(91 7)	(101 40)	(102 91)
(103 27)	(104 112)	(105 8)	(116 28)	(117 39)
(118 652)	(119 67)	(120 20)	(130 5)	(131 14)
(132 60)	(133 82)	(134 446)	(135 36)	(136 12)
(145 6)	(147 89)	(148 54)	(149 12)	(162 30)
(174 5)	(208 5)	(221 20)	(228 7)	(237 17)

NAME:13C_1220.5_1313EC11_Valine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:122001-11-1

RI:1221

RT:5.509

NUM PEAKS: 25

(70	12)	(72	35)	(73	981)	(74	127)	(75	355)
(76	99)	(79	48)	(87	43)	(88	19)	(100	21)
(101	112)	(102	28)	(103	16)	(104	13)	(117	35)
(131	23)	(132	66)	(133	58)	(147	192)	(148	1000)
(149	100)	(150	39)	(161	15)	(220	75)	(222	41)

NAME:13C_1314.0_1313EC16_Isoleucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:132002-11-1

RI:1314

RT:6.570

NUM PEAKS: 27

(90	6)	(91	25)	(101	80)	(118	8)	(132	49)
(158	10)	(160	9)	(161	9)	(162	47)	(163	1000)
(164	88)	(165	30)	(196	1)	(203	1)	(204	2)
(205	6)	(207	5)	(215	1)	(220	52)	(236	2)
(237	37)	(238	9)	(239	3)	(266	8)	(267	2)
(268	1)	(347	1)						

NAME:13C_1354.8_1313EC11_Glyceric acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:135003-11-1

RI:1355

RT:7.049

NUM PEAKS: 14

(73	1000)	(74	82)	(103	176)	(104	107)	(118	23)
(119	71)	(131	35)	(132	50)	(133	190)	(147	359)
(148	57)	(191	224)	(207	37)	(294	62)		

NAME:13C_1372.0_1313EC11_Fumaric acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:137001-11-1

RI:1372

RT:7.282

NUM PEAKS: 124

(70	21)	(71	81)	(72	7)	(73	1000)	(74	112)
(75	527)	(76	32)	(80	9)	(81	21)	(82	27)
(83	114)	(84	43)	(85	152)	(86	42)	(94	12)
(95	11)	(97	17)	(98	5)	(101	15)	(103	9)
(104	3)	(105	14)	(106	4)	(108	10)	(109	8)
(110	16)	(111	7)	(112	17)	(113	5)	(114	6)
(115	68)	(116	21)	(117	56)	(118	9)	(119	4)
(124	7)	(127	27)	(128	13)	(129	24)	(130	19)
(131	28)	(132	8)	(133	137)	(134	25)	(135	16)
(136	4)	(139	10)	(141	4)	(142	6)	(143	111)
(144	25)	(145	22)	(146	90)	(147	792)	(148	127)
(149	90)	(150	17)	(151	4)	(152	14)	(155	43)
(156	24)	(157	40)	(158	15)	(159	56)	(160	1)
(165	3)	(167	3)	(170	4)	(171	41)	(172	16)
(176	1)	(177	12)	(178	6)	(180	2)	(185	1)
(186	2)	(188	3)	(190	3)	(191	12)	(192	7)
(193	2)	(195	9)	(198	1)	(199	12)	(200	3)
(202	8)	(206	1)	(209	4)	(210	6)	(214	2)
(216	2)	(217	22)	(218	11)	(219	5)	(220	15)

(221	8)	(225	7)	(228	3)	(229	2)	(230	4)
(231	3)	(232	1)	(234	6)	(238	3)	(240	6)
(244	12)	(245	437)	(246	91)	(247	32)	(248	28)
(249	324)	(250	48)	(251	15)	(253	2)	(254	6)
(259	2)	(260	4)	(264	1)	(265	3)	(269	10)
(270	6)	(271	12)	(272	2)	(273	2)		

NAME:13C 1449.3 1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144007-11-1

RI:1449

RT:8.163

NUM PEAKS: 308

(72	69)	(73	1000)	(74	220)	(75	423)	(76	73)
(77	47)	(79	38)	(82	2)	(83	12)	(84	4)
(85	17)	(86	16)	(87	9)	(88	15)	(89	27)
(90	16)	(91	12)	(92	25)	(93	9)	(94	8)
(97	6)	(98	19)	(100	19)	(101	47)	(102	65)
(103	41)	(104	50)	(105	18)	(109	14)	(110	7)
(111	10)	(112	11)	(115	32)	(116	11)	(117	23)
(118	202)	(119	154)	(120	14)	(121	21)	(122	16)
(126	3)	(128	8)	(129	5)	(130	14)	(131	23)
(132	207)	(133	73)	(134	9)	(135	12)	(137	11)
(138	12)	(139	1)	(140	15)	(142	32)	(143	4)
(146	21)	(147	328)	(148	57)	(149	35)	(151	8)
(152	2)	(155	10)	(156	29)	(158	15)	(159	15)
(160	15)	(162	27)	(163	327)	(164	27)	(165	10)
(167	2)	(168	5)	(169	3)	(171	1)	(174	6)
(175	22)	(176	14)	(177	2)	(179	4)	(180	10)
(181	7)	(182	11)	(184	9)	(186	27)	(187	9)
(190	2)	(192	1)	(193	12)	(195	15)	(196	5)
(197	17)	(200	27)	(201	3)	(202	22)	(204	13)
(205	25)	(206	1)	(207	9)	(212	8)	(214	8)
(216	6)	(223	6)	(226	18)	(229	7)	(232	5)
(234	13)	(235	13)	(236	25)	(237	17)	(238	1)
(241	2)	(242	5)	(246	4)	(249	42)	(250	1)
(252	17)	(255	11)	(256	2)	(257	19)	(258	27)
(259	2)	(266	12)	(269	5)	(272	6)	(276	19)
(277	3)	(278	9)	(281	1)	(283	24)	(284	8)
(288	6)	(289	2)	(290	7)	(294	7)	(295	3)
(298	4)	(312	13)	(313	1)	(314	7)	(315	1)
(321	5)	(322	4)	(326	7)	(327	18)	(328	7)
(329	6)	(330	2)	(333	7)	(334	18)	(335	17)
(336	8)	(337	3)	(338	4)	(342	18)	(344	9)
(345	18)	(346	5)	(349	13)	(350	5)	(352	6)
(353	7)	(354	12)	(356	20)	(357	11)	(358	21)
(361	15)	(362	14)	(363	6)	(365	8)	(366	19)
(367	9)	(368	18)	(370	1)	(371	2)	(372	5)
(373	11)	(375	16)	(379	6)	(380	6)	(381	22)
(382	2)	(383	18)	(384	8)	(386	11)	(387	3)
(388	7)	(389	18)	(390	10)	(393	8)	(394	6)
(396	10)	(397	8)	(400	22)	(401	2)	(402	18)
(404	11)	(405	10)	(406	4)	(407	7)	(409	11)
(410	1)	(413	1)	(414	21)	(415	5)	(416	26)
(417	13)	(419	2)	(422	5)	(424	9)	(425	1)
(426	15)	(429	10)	(431	12)	(432	8)	(433	10)
(436	13)	(438	23)	(441	8)	(444	27)	(445	8)
(447	3)	(448	6)	(449	12)	(452	18)	(453	15)
(454	11)	(457	13)	(459	4)	(460	24)	(461	16)
(462	1)	(464	8)	(466	18)	(467	5)	(471	12)

(472	15)	(475	31)	(476	3)	(477	1)	(481	10)
(482	13)	(483	2)	(486	2)	(487	3)	(488	14)
(489	29)	(490	21)	(492	1)	(493	3)	(494	18)
(496	3)	(499	17)	(500	7)	(502	6)	(503	3)
(506	24)	(507	9)	(508	1)	(509	28)	(511	12)
(512	6)	(513	3)	(517	11)	(518	14)	(519	1)
(523	12)	(525	14)	(527	12)	(530	23)	(531	19)
(533	4)	(534	14)	(535	2)	(537	9)	(538	6)
(539	4)	(541	15)	(542	5)	(548	12)	(553	13)
(554	5)	(559	3)	(560	4)	(563	14)	(564	3)
(565	7)	(568	2)	(569	11)	(571	11)	(573	3)
(574	4)	(575	12)	(576	4)	(578	4)	(579	4)
(580	5)	(582	6)	(583	9)	(584	1)	(585	1)
(586	1)	(587	6)	(591	1)	(592	17)	(593	4)
(595	3)	(596	3)	(597	1)				

NAME:13C_1726.4_1313EC11_Fucose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173002-11-1

RI:1726

RT:10.512

NUM PEAKS: 37

(72	106)	(73	999)	(103	153)	(106	69)	(116	32)
(117	68)	(118	45)	(119	1000)	(120	73)	(131	164)
(134	51)	(135	40)	(137	33)	(146	50)	(148	204)
(149	120)	(175	25)	(190	63)	(191	164)	(192	128)
(193	40)	(205	27)	(219	34)	(222	65)	(235	26)
(249	25)	(250	123)	(260	14)	(294	32)	(309	19)
(311	36)	(322	52)	(324	40)	(337	33)	(398	20)
(500	17)	(537	15)						

NAME:13C_1785.2_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179001-11-1

RI:1785

RT:10.978

NUM PEAKS: 337

(72	18)	(73	1000)	(74	72)	(75	49)	(76	9)
(78	3)	(82	3)	(86	3)	(88	3)	(89	5)
(90	18)	(91	12)	(92	2)	(94	2)	(96	1)
(97	2)	(103	52)	(104	225)	(105	24)	(106	9)
(107	2)	(108	2)	(109	2)	(115	8)	(117	3)
(118	9)	(119	58)	(120	6)	(121	4)	(122	2)
(128	1)	(129	3)	(131	21)	(132	63)	(133	93)
(134	29)	(135	13)	(138	2)	(140	2)	(141	1)
(144	2)	(145	9)	(146	29)	(147	213)	(148	42)
(149	34)	(150	7)	(151	4)	(152	1)	(154	1)
(155	3)	(157	1)	(159	2)	(161	10)	(162	3)
(163	2)	(164	3)	(165	4)	(166	1)	(167	3)
(168	2)	(176	3)	(177	8)	(178	3)	(179	4)
(180	3)	(181	6)	(182	2)	(183	2)	(184	2)
(187	1)	(188	2)	(189	4)	(191	47)	(192	22)
(193	9)	(195	7)	(196	1)	(197	2)	(199	2)
(200	2)	(202	1)	(205	4)	(206	51)	(207	41)
(208	9)	(209	4)	(210	4)	(211	12)	(213	3)
(214	2)	(215	1)	(216	1)	(217	2)	(218	2)
(219	5)	(220	131)	(221	42)	(222	15)	(223	3)
(224	1)	(228	3)	(231	1)	(233	3)	(234	3)
(238	1)	(239	2)	(240	1)	(242	3)	(243	3)
(244	2)	(245	2)	(246	1)	(247	1)	(248	1)

94

(249	3)	(252	2)	(253	2)	(254	2)	(256	3)
(257	2)	(259	3)	(261	1)	(262	9)	(263	4)
(264	5)	(266	3)	(269	2)	(272	1)	(273	1)
(274	2)	(275	2)	(276	2)	(277	2)	(279	14)
(280	5)	(281	1)	(282	2)	(284	1)	(285	4)
(286	2)	(287	2)	(288	1)	(291	1)	(292	3)
(293	11)	(294	137)	(295	38)	(296	18)	(297	3)
(298	4)	(299	6)	(300	4)	(301	4)	(302	2)
(303	1)	(305	1)	(306	1)	(307	5)	(308	20)
(309	8)	(310	19)	(311	5)	(312	3)	(315	3)
(316	2)	(317	2)	(318	2)	(319	2)	(320	1)
(322	1)	(323	3)	(324	3)	(330	2)	(332	3)
(333	2)	(335	3)	(336	10)	(337	15)	(338	6)
(339	3)	(340	2)	(343	1)	(345	2)	(346	2)
(348	2)	(349	3)	(351	6)	(352	5)	(353	3)
(354	1)	(358	2)	(360	2)	(362	2)	(363	2)
(364	2)	(365	1)	(366	2)	(369	2)	(370	1)
(372	3)	(373	4)	(374	3)	(375	2)	(382	3)
(383	2)	(384	2)	(386	2)	(387	3)	(389	2)
(390	3)	(391	2)	(392	2)	(394	2)	(396	2)
(397	2)	(398	1)	(399	2)	(400	1)	(404	2)
(405	2)	(406	2)	(408	2)	(410	1)	(411	1)
(412	1)	(416	2)	(420	1)	(421	2)	(422	2)
(423	2)	(424	3)	(425	2)	(426	5)	(427	3)
(428	1)	(432	2)	(433	2)	(434	2)	(435	3)
(436	2)	(438	2)	(439	2)	(440	1)	(441	2)
(442	2)	(444	2)	(445	3)	(446	2)	(447	2)
(448	3)	(449	2)	(450	2)	(451	1)	(452	2)
(453	2)	(454	2)	(455	1)	(456	2)	(457	2)
(458	1)	(459	1)	(460	2)	(461	2)	(462	2)
(463	2)	(464	2)	(465	3)	(467	1)	(468	1)
(469	1)	(470	2)	(472	2)	(473	2)	(474	2)
(475	1)	(478	2)	(480	2)	(481	2)	(483	2)
(485	2)	(486	2)	(487	2)	(488	2)	(489	1)
(490	2)	(491	2)	(492	1)	(496	1)	(497	1)
(498	2)	(499	2)	(500	2)	(502	2)	(503	1)
(504	2)	(506	1)	(508	2)	(510	1)	(511	2)
(512	2)	(513	1)	(514	2)	(515	3)	(516	4)
(517	3)	(518	2)	(519	2)	(520	2)	(521	1)
(522	2)	(523	2)	(525	3)	(526	2)	(527	2)
(530	2)	(531	1)	(533	2)	(534	2)	(535	2)
(539	2)	(540	2)	(541	3)	(544	1)	(545	2)
(546	1)	(548	1)	(552	2)	(555	1)	(556	1)
(559	1)	(564	1)	(570	1)	(571	1)	(572	1)
(573	1)	(575	1)						

NAME:13C_1802.7_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180002-11-1

RI:1803

RT:11.114

NUM PEAKS: 85

(72	9)	(73	1000)	(74	103)	(75	108)	(76	12)
(87	5)	(90	8)	(92	1)	(94	1)	(102	4)
(103	21)	(104	13)	(114	5)	(116	2)	(118	9)
(119	25)	(130	1)	(131	27)	(132	46)	(133	32)
(134	6)	(135	7)	(136	1)	(140	4)	(144	2)
(145	26)	(146	21)	(147	102)	(148	15)	(149	11)
(157	2)	(159	1)	(161	19)	(174	9)	(177	1)
(186	1)	(188	2)	(189	2)	(190	1)	(191	15)

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(192	35)	(193	8)	(194	3)	(207	9)	(208	2)
(218	2)	(219	10)	(220	34)	(221	24)	(233	6)
(234	3)	(242	1)	(248	2)	(249	1)	(250	3)
(251	4)	(252	1)	(260	1)	(261	2)	(262	49)
(263	6)	(264	3)	(278	6)	(279	4)	(292	1)
(294	3)	(295	12)	(296	1)	(297	1)	(307	6)
(308	1)	(323	6)	(324	1)	(352	5)	(353	2)
(354	2)	(368	2)	(369	1)	(429	1)	(441	7)
(442	30)	(443	14)	(444	5)	(512	1)	(564	1)

NAME:13C_1805.7_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181004-11-1

RI:1806

RT:11.136

NUM PEAKS: 125

(70	10)	(71	8)	(72	12)	(73	1000)	(74	100)
(75	144)	(76	13)	(77	8)	(81	3)	(82	5)
(83	16)	(84	5)	(85	5)	(86	11)	(87	5)
(90	10)	(91	5)	(92	1)	(93	1)	(94	1)
(95	2)	(96	3)	(97	15)	(98	3)	(100	2)
(101	3)	(102	4)	(103	17)	(104	28)	(109	1)
(110	1)	(111	7)	(112	2)	(114	6)	(115	3)
(116	5)	(117	5)	(118	10)	(119	41)	(120	3)
(121	1)	(124	2)	(125	3)	(129	7)	(130	2)
(131	22)	(132	50)	(133	34)	(134	7)	(135	6)
(136	1)	(140	5)	(141	1)	(144	3)	(145	27)
(146	15)	(147	110)	(148	18)	(149	22)	(150	2)
(151	1)	(152	2)	(153	1)	(154	1)	(159	1)
(160	4)	(161	19)	(174	15)	(176	2)	(179	1)
(188	3)	(189	2)	(190	2)	(191	13)	(196	2)
(201	2)	(204	3)	(214	1)	(217	2)	(218	5)
(219	15)	(220	98)	(221	34)	(222	8)	(223	2)
(224	1)	(233	7)	(234	6)	(237	1)	(248	3)
(249	1)	(251	3)	(260	1)	(261	4)	(262	56)
(263	8)	(264	5)	(265	2)	(276	1)	(278	4)
(279	4)	(280	1)	(294	2)	(295	8)	(296	2)
(307	8)	(308	3)	(309	1)	(317	2)	(323	7)
(324	2)	(336	1)	(351	1)	(352	7)	(353	2)
(354	2)	(368	3)	(369	1)	(370	1)	(440	1)
(441	10)	(442	40)	(443	17)	(444	8)	(445	1)

NAME:13C_1842.0_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184002-11-1

RI:1842

RT:11.427

NUM PEAKS: 140

(70	11)	(71	8)	(72	30)	(73	1000)	(74	101)
(75	178)	(76	10)	(77	17)	(78	3)	(79	4)
(85	75)	(86	6)	(87	19)	(88	5)	(89	6)
(90	15)	(91	3)	(92	1)	(93	4)	(94	1)
(95	3)	(97	1)	(98	6)	(99	25)	(100	23)
(101	28)	(102	16)	(103	55)	(104	44)	(105	9)
(106	2)	(113	3)	(114	9)	(115	13)	(116	8)
(117	15)	(118	16)	(119	72)	(120	5)	(121	1)
(127	1)	(129	10)	(130	10)	(131	23)	(133	56)
(134	12)	(135	4)	(141	11)	(142	6)	(143	8)
(144	5)	(145	16)	(146	13)	(147	171)	(148	29)
(157	31)	(158	28)	(159	10)	(160	4)	(161	7)

(162	14)	(163	1)	(170	4)	(171	19)	(172	72)
(173	526)	(174	227)	(175	32)	(176	6)	(177	6)
(178	2)	(179	1)	(185	3)	(186	3)	(187	7)
(188	2)	(189	2)	(190	2)	(191	5)	(192	15)
(193	3)	(198	1)	(199	1)	(200	1)	(201	13)
(202	3)	(203	2)	(204	1)	(209	1)	(211	1)
(212	1)	(213	5)	(214	1)	(215	2)	(216	1)
(217	1)	(219	2)	(220	19)	(221	5)	(222	3)
(231	2)	(232	2)	(243	6)	(244	9)	(245	25)
(246	29)	(247	8)	(248	1)	(260	3)	(261	5)
(262	23)	(263	5)	(264	1)	(266	3)	(270	3)
(273	1)	(274	1)	(275	8)	(276	3)	(285	1)
(289	1)	(290	13)	(291	3)	(307	3)	(308	1)
(334	6)	(335	2)	(336	2)	(337	1)	(352	2)
(353	1)	(365	5)	(366	1)	(374	1)	(380	9)
(381	2)	(441	3)	(442	15)	(443	6)	(444	1)

NAME:13C_1847.4_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185003-11-1

RI:1847

RT:11.461

NUM PEAKS: 205

(71	111)	(74	923)	(75	999)	(76	60)	(77	33)
(80	5)	(86	69)	(87	109)	(88	35)	(89	133)
(90	149)	(91	23)	(92	9)	(94	6)	(96	11)
(101	170)	(102	109)	(104	542)	(105	78)	(106	25)
(108	5)	(112	16)	(115	158)	(116	59)	(118	157)
(120	49)	(121	25)	(130	87)	(131	346)	(132	605)
(134	142)	(135	76)	(136	10)	(138	6)	(139	5)
(144	76)	(146	151)	(150	38)	(151	22)	(153	4)
(155	15)	(159	84)	(160	1000)	(161	714)	(162	190)
(163	178)	(164	33)	(165	11)	(166	5)	(167	3)
(168	4)	(178	44)	(179	14)	(184	7)	(188	14)
(189	37)	(190	27)	(191	374)	(196	3)	(197	7)
(198	11)	(203	40)	(204	47)	(205	61)	(207	249)
(209	23)	(210	4)	(212	8)	(215	10)	(217	22)
(218	40)	(223	30)	(224	8)	(226	4)	(229	7)
(230	13)	(232	73)	(233	49)	(234	99)	(235	97)
(236	35)	(237	22)	(238	9)	(239	4)	(248	150)
(249	72)	(250	32)	(251	60)	(252	12)	(253	7)
(254	4)	(256	3)	(261	12)	(263	18)	(269	8)
(271	4)	(272	5)	(274	14)	(277	58)	(278	29)
(280	10)	(281	10)	(282	5)	(289	13)	(292	10)
(294	35)	(295	12)	(296	5)	(297	3)	(298	5)
(306	16)	(307	22)	(319	5)	(321	21)	(322	271)
(323	212)	(324	81)	(325	22)	(326	8)	(331	5)
(335	20)	(338	14)	(339	6)	(340	4)	(341	6)
(342	5)	(343	4)	(346	5)	(347	6)	(348	5)
(349	7)	(350	11)	(351	55)	(352	46)	(353	22)
(354	11)	(359	4)	(362	6)	(363	3)	(368	11)
(369	6)	(372	6)	(377	4)	(383	5)	(384	5)
(387	4)	(388	5)	(391	5)	(396	8)	(397	8)
(398	8)	(404	3)	(405	6)	(410	3)	(412	9)
(413	5)	(416	4)	(424	7)	(425	33)	(426	13)
(427	6)	(431	3)	(434	3)	(438	5)	(439	6)
(440	4)	(441	10)	(444	10)	(447	6)	(448	5)
(454	4)	(455	3)	(459	4)	(461	5)	(462	5)
(463	4)	(466	7)	(467	5)	(469	4)	(470	4)
(477	5)	(489	3)	(492	2)	(496	5)	(499	3)

(504	4)	(521	3)	(527	4)	(538	2)	(541	3)
(542	4)	(545	3)	(551	2)	(553	3)	(556	2)
(559	2)	(560	3)	(563	3)	(567	2)	(569	4)
(570	2)	(572	4)	(573	2)	(588	3)	(590	2)

NAME:13C_1869.1_1313EC11_Fructose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187002-11-1

RI:1869

RT:11.620

NUM PEAKS: 110

(72	19)	(73	1000)	(74	96)	(76	3)	(85	19)
(86	5)	(88	5)	(89	19)	(90	19)	(91	3)
(92	1)	(102	6)	(103	35)	(104	174)	(105	20)
(106	7)	(107	1)	(116	9)	(117	9)	(118	7)
(119	50)	(120	5)	(121	2)	(131	26)	(132	25)
(133	55)	(134	23)	(135	8)	(136	1)	(145	7)
(146	7)	(147	206)	(148	38)	(149	23)	(150	2)
(151	1)	(160	4)	(161	5)	(163	4)	(164	2)
(165	1)	(175	2)	(176	9)	(177	8)	(178	4)
(179	1)	(188	2)	(190	2)	(191	15)	(192	8)
(193	3)	(194	1)	(203	6)	(204	3)	(205	3)
(206	16)	(207	18)	(208	5)	(209	2)	(210	1)
(217	4)	(218	2)	(219	5)	(220	80)	(221	17)
(222	8)	(223	1)	(233	2)	(234	2)	(235	1)
(236	1)	(237	1)	(249	1)	(250	1)	(261	2)
(262	1)	(263	1)	(264	1)	(265	2)	(266	3)
(267	1)	(268	1)	(277	1)	(278	1)	(279	7)
(280	3)	(281	2)	(282	1)	(291	1)	(293	1)
(294	2)	(295	1)	(296	1)	(305	1)	(306	1)
(307	1)	(308	1)	(309	2)	(310	28)	(311	7)
(312	3)	(335	1)	(337	1)	(338	2)	(339	1)
(354	1)	(367	1)	(368	4)	(369	2)	(370	1)

NAME:13C_2137.1_1313EC16_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:214003-11-1

RI:2137

RT:13.366

NUM PEAKS: 65

(72	12)	(73	1000)	(74	81)	(75	68)	(85	12)
(86	11)	(87	15)	(89	32)	(90	19)	(99	6)
(101	4)	(102	10)	(103	21)	(104	181)	(105	15)
(106	7)	(116	15)	(117	10)	(118	10)	(119	67)
(120	4)	(131	25)	(132	77)	(133	50)	(134	46)
(135	7)	(145	4)	(146	12)	(147	244)	(148	35)
(149	18)	(151	5)	(158	6)	(161	67)	(162	7)
(169	3)	(173	19)	(174	5)	(176	8)	(177	8)
(191	25)	(192	11)	(203	6)	(204	5)	(206	28)
(207	120)	(208	20)	(220	74)	(233	14)	(235	8)
(236	3)	(250	4)	(265	6)	(274	3)	(279	7)
(308	4)	(322	12)	(323	118)	(324	35)	(325	14)
(422	4)	(449	3)	(466	5)	(478	3)	(590	3)

NAME:13C_2246.0_1313EC16_Octadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:225002-11-1

RI:2246

RT:14.010

NUM PEAKS: 87

98

(72	70)	(75	1000)	(76	106)	(77	52)	(78	7)
(88	25)	(89	82)	(90	9)	(91	31)	(92	9)
(93	17)	(94	3)	(106	20)	(107	10)	(118	135)
(119	540)	(120	41)	(121	30)	(125	3)	(128	7)
(132	504)	(134	364)	(135	69)	(136	17)	(146	22)
(148	153)	(149	31)	(151	6)	(158	4)	(160	7)
(162	12)	(163	23)	(170	3)	(178	3)	(187	12)
(192	20)	(194	4)	(205	3)	(208	35)	(214	4)
(219	4)	(220	12)	(223	9)	(233	4)	(234	5)
(235	5)	(237	6)	(246	5)	(252	7)	(253	8)
(254	3)	(260	3)	(265	4)	(268	13)	(269	3)
(279	3)	(284	3)	(308	3)	(313	6)	(314	7)
(319	4)	(323	4)	(328	6)	(334	3)	(337	4)
(357	15)	(358	28)	(359	97)	(360	19)	(367	3)
(374	18)	(395	3)	(400	5)	(421	4)	(427	3)
(434	3)	(436	3)	(443	3)	(444	5)	(467	4)
(488	3)	(491	4)	(499	5)	(506	4)	(507	4)
(520	3)	(535	3)						

NAME:13C_2327.6_1313EC16_Glucose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:233002-11-1

RT:2328

RT:14.442

NUM PEAKS: 51

(72	20)	(73	1000)	(74	79)	(75	77)	(80	17)
(87	19)	(89	36)	(101	18)	(103	46)	(104	30)
(105	39)	(116	21)	(118	25)	(119	18)	(131	30)
(132	72)	(133	77)	(134	24)	(135	29)	(142	10)
(146	20)	(147	150)	(148	24)	(161	50)	(162	85)
(175	12)	(191	14)	(193	18)	(206	17)	(207	20)
(211	37)	(220	32)	(225	20)	(260	7)	(275	9)
(278	14)	(283	12)	(299	100)	(300	30)	(314	15)
(315	41)	(317	12)	(332	13)	(359	36)	(360	18)
(386	32)	(387	113)	(388	46)	(389	25)	(476	10)
(541	11)								

NAME:13C_2748.0_1313EC16_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:274002-11-1

RI:2748

RT:16.667

NUM PEAKS: 110

(71	5)	(72	15)	(73	1000)	(74	83)	(85	5)
(86	23)	(87	11)	(88	4)	(89	6)	(90	13)
(100	3)	(101	7)	(102	9)	(103	22)	(104	181)
(105	19)	(106	7)	(114	4)	(115	17)	(116	11)
(117	8)	(118	16)	(119	58)	(120	6)	(130	4)
(131	24)	(132	151)	(133	72)	(134	16)	(135	7)
(144	6)	(145	8)	(146	23)	(147	268)	(148	48)
(149	34)	(150	4)	(158	6)	(159	5)	(160	31)
(161	26)	(162	5)	(163	4)	(164	4)	(173	6)
(174	103)	(175	15)	(176	12)	(177	10)	(178	6)
(189	10)	(190	4)	(191	42)	(192	254)	(193	46)
(194	21)	(204	3)	(205	10)	(206	92)	(207	34)
(208	12)	(209	3)	(218	5)	(219	8)	(220	148)
(221	48)	(222	20)	(223	5)	(232	4)	(233	12)
(234	9)	(235	14)	(236	10)	(237	4)	(246	5)
(247	5)	(248	52)	(249	18)	(250	9)	(251	4)
(261	3)	(262	6)	(263	3)	(264	5)	(266	4)

(267	5)	(276	4)	(277	48)	(278	10)	(279	10)
(280	5)	(293	5)	(294	13)	(295	5)	(308	11)
(309	5)	(310	3)	(322	6)	(323	17)	(324	7)
(325	3)	(336	15)	(337	9)	(338	4)	(366	27)
(367	211)	(368	69)	(369	33)	(370	7)	(441	3)

NAME:13C_3269.3_1313EC16_Ergosterol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:327001-11-1

RI:3269

RT:19.000

NUM PEAKS: 216

(70	52)	(71	91)	(72	223)	(73	1000)	(74	477)
(75	395)	(76	47)	(77	13)	(80	16)	(81	15)
(82	35)	(83	92)	(84	49)	(85	151)	(86	68)
(87	273)	(88	97)	(89	98)	(90	9)	(91	12)
(92	5)	(93	7)	(94	9)	(95	8)	(96	28)
(97	32)	(98	180)	(99	31)	(100	117)	(101	39)
(102	105)	(103	45)	(104	27)	(105	5)	(106	5)
(107	3)	(109	6)	(110	13)	(111	24)	(112	28)
(113	137)	(114	23)	(115	78)	(116	34)	(117	61)
(118	34)	(119	12)	(120	3)	(122	6)	(123	15)
(124	99)	(125	30)	(126	89)	(127	43)	(128	195)
(129	14)	(130	32)	(131	21)	(132	94)	(133	82)
(134	168)	(135	18)	(136	21)	(137	59)	(138	166)
(139	132)	(140	42)	(141	123)	(142	22)	(143	51)
(144	11)	(145	22)	(146	12)	(147	23)	(148	112)
(149	15)	(150	20)	(151	30)	(152	159)	(153	114)
(154	271)	(155	58)	(156	161)	(157	20)	(158	42)
(159	9)	(160	26)	(161	7)	(162	10)	(163	16)
(164	43)	(165	59)	(166	51)	(167	133)	(168	76)
(169	241)	(170	70)	(171	133)	(172	12)	(173	13)
(174	16)	(175	37)	(176	12)	(177	17)	(178	57)
(179	30)	(180	55)	(181	44)	(182	111)	(183	46)
(184	95)	(185	17)	(186	24)	(187	6)	(188	8)
(189	13)	(190	7)	(191	8)	(192	21)	(193	26)
(194	23)	(195	57)	(196	40)	(197	102)	(198	31)
(199	74)	(200	11)	(201	12)	(202	9)	(203	6)
(204	10)	(205	5)	(206	7)	(207	7)	(209	21)
(211	40)	(212	102)	(213	32)	(214	63)	(215	7)
(216	13)	(217	3)	(218	4)	(219	5)	(220	4)
(221	4)	(222	4)	(223	10)	(224	14)	(225	46)
(226	42)	(227	138)	(228	24)	(229	46)	(230	4)
(231	3)	(232	8)	(233	3)	(237	3)	(238	8)
(239	10)	(240	26)	(241	17)	(242	34)	(243	32)
(244	20)	(245	4)	(256	18)	(257	30)	(258	5)
(259	3)	(268	7)	(269	14)	(270	49)	(271	34)
(272	93)	(273	5)	(284	5)	(285	14)	(286	6)
(287	7)	(298	3)	(299	4)	(300	9)	(301	7)
(302	3)	(304	3)	(314	5)	(315	8)	(316	3)
(330	3)	(332	3)	(346	4)	(347	3)	(348	3)
(349	5)	(358	5)	(359	18)	(360	40)	(361	104)
(362	52)	(363	8)	(386	7)	(387	24)	(388	58)
(389	146)	(390	68)	(391	9)	(403	8)	(404	19)
(405	38)	(406	18)	(494	13)	(495	27)	(496	16)
(497	4)								

NAME:13C_2109.4_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211004-11-1

100

RI:2109

RT:13.190

NUM PEAKS: 70

(72	29)	(73	1000)	(74	86)	(75	98)	(77	12)
(89	46)	(90	11)	(99	6)	(102	16)	(103	59)
(105	25)	(115	14)	(116	17)	(117	15)	(118	20)
(119	22)	(130	9)	(131	33)	(132	122)	(133	81)
(134	20)	(135	19)	(137	8)	(146	11)	(147	158)
(148	29)	(149	21)	(151	8)	(157	4)	(161	34)
(162	45)	(163	16)	(164	6)	(165	4)	(173	12)
(177	7)	(181	10)	(189	6)	(191	12)	(192	10)
(193	13)	(195	10)	(203	10)	(205	11)	(206	12)
(207	27)	(211	57)	(212	10)	(219	12)	(220	143)
(221	32)	(222	11)	(225	14)	(227	16)	(262	3)
(277	10)	(298	11)	(299	114)	(300	36)	(301	17)
(314	17)	(315	176)	(316	50)	(317	25)	(359	17)
(360	6)	(367	5)	(403	14)	(404	7)	(462	12)

NAME:13C_2114.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211003-11-1

RI:2114

RT:13.220

NUM PEAKS: 23

(70	8)	(73	1000)	(74	98)	(75	120)	(87	21)
(98	8)	(103	55)	(116	17)	(131	26)	(132	109)
(133	75)	(146	11)	(147	153)	(173	10)	(175	76)
(176	25)	(220	103)	(221	20)	(285	6)	(299	112)
(315	140)	(316	37)	(415	6)				

NAME:13C_2125.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213003-11-1

RI:2125

RT:13.290

NUM PEAKS: 42

(72	22)	(73	959)	(74	81)	(75	61)	(87	150)
(89	19)	(90	21)	(101	69)	(102	21)	(103	35)
(104	78)	(117	12)	(119	54)	(130	26)	(131	30)
(132	38)	(133	40)	(134	14)	(145	15)	(147	176)
(148	30)	(151	13)	(160	16)	(162	25)	(175	1000)
(176	174)	(177	74)	(187	8)	(189	17)	(191	17)
(192	23)	(206	36)	(207	33)	(220	41)	(221	16)
(249	8)	(298	14)	(310	7)	(369	10)	(454	12)
(511	13)	(532	12)						

NAME:13C_2131.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213001-11-1

RI:2131

RT:13.328

NUM PEAKS: 160

(72	17)	(73	1000)	(74	76)	(75	67)	(85	14)
(86	6)	(87	16)	(88	6)	(89	44)	(90	24)
(92	3)	(95	3)	(96	3)	(97	5)	(100	5)
(101	13)	(102	17)	(103	21)	(104	153)	(105	23)
(106	6)	(107	5)	(110	4)	(115	9)	(116	27)
(117	7)	(118	6)	(119	73)	(120	13)	(128	4)
(131	28)	(132	102)	(133	55)	(134	20)	(135	7)
(137	4)	(140	5)	(145	9)	(146	12)	(147	250)

101

(148	40)	(149	27)	(151	6)	(154	3)	(158	5)
(161	76)	(162	9)	(163	10)	(164	4)	(165	4)
(166	5)	(167	3)	(173	8)	(174	4)	(176	7)
(177	9)	(178	8)	(182	3)	(186	4)	(187	5)
(189	5)	(191	30)	(192	18)	(198	3)	(203	6)
(205	4)	(206	36)	(207	122)	(208	19)	(209	12)
(219	9)	(220	91)	(226	4)	(228	3)	(233	22)
(235	6)	(239	3)	(241	4)	(250	3)	(251	4)
(252	4)	(253	3)	(255	3)	(259	6)	(261	7)
(262	5)	(264	8)	(265	31)	(266	10)	(275	4)
(276	3)	(279	5)	(287	3)	(288	6)	(289	4)
(290	3)	(293	4)	(294	10)	(302	4)	(305	3)
(307	3)	(308	5)	(309	6)	(310	8)	(312	4)
(319	5)	(320	6)	(322	20)	(323	145)	(324	43)
(325	17)	(329	4)	(333	5)	(334	5)	(336	5)
(337	5)	(338	7)	(339	5)	(342	3)	(349	5)
(352	5)	(358	3)	(359	3)	(361	3)	(362	4)
(376	3)	(377	5)	(378	4)	(379	5)	(380	3)
(384	4)	(389	3)	(401	4)	(409	3)	(412	3)
(417	4)	(425	3)	(432	4)	(433	5)	(434	4)
(441	3)	(448	6)	(455	5)	(456	5)	(462	5)
(463	5)	(465	3)	(467	4)	(468	4)	(478	3)
(479	3)	(500	5)	(501	5)	(505	4)	(525	5)
(528	5)	(534	3)	(536	3)	(540	3)	(567	3)

NAME:13C_2155.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216003-11-1

RI:2155

RT:13.481

NUM PEAKS: 35

(73	1000)	(74	95)	(86	9)	(87	35)	(90	22)
(91	40)	(104	176)	(115	25)	(118	20)	(119	84)
(129	18)	(131	31)	(132	55)	(133	50)	(145	24)
(147	211)	(148	36)	(149	42)	(157	10)	(161	17)
(162	14)	(174	8)	(176	18)	(177	7)	(178	38)
(192	6)	(203	21)	(204	15)	(207	55)	(220	75)
(221	17)	(235	25)	(249	9)	(352	25)	(441	6)

NAME:13C_2162.2_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216002-11-1

RI:2162

RT:13.526

NUM PEAKS: 93

(72	17)	(73	1000)	(74	83)	(75	56)	(86	6)
(87	137)	(88	11)	(89	26)	(90	15)	(100	5)
(101	90)	(102	14)	(103	34)	(104	157)	(105	16)
(106	6)	(115	7)	(116	8)	(117	13)	(118	8)
(119	61)	(120	5)	(129	5)	(130	15)	(131	23)
(132	38)	(133	40)	(134	13)	(135	4)	(143	3)
(145	11)	(146	9)	(147	186)	(148	31)	(149	16)
(157	5)	(159	8)	(161	16)	(173	30)	(174	12)
(175	250)	(176	43)	(177	20)	(178	3)	(187	13)
(188	5)	(189	5)	(191	22)	(192	8)	(201	4)
(202	6)	(203	6)	(204	4)	(205	3)	(206	16)
(207	45)	(208	8)	(217	8)	(218	4)	(219	12)
(220	96)	(221	20)	(222	8)	(233	5)	(245	19)
(260	4)	(261	6)	(273	7)	(274	18)	(275	5)
(276	3)	(279	6)	(290	16)	(291	6)	(294	3)

102

(304	5)	(305	4)	(306	4)	(307	3)	(308	8)
(309	4)	(310	17)	(311	5)	(318	10)	(319	12)
(320	5)	(323	6)	(335	6)	(349	11)	(350	3)
(435	3)	(525	5)	(526	4)				

NAME:13C_2168.8_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:217002-11-1

RI:2169

RT:13.568

NUM PEAKS: 18

(73	1000)	(74	83)	(75	81)	(87	57)	(101	31)
(103	14)	(132	37)	(133	38)	(145	24)	(147	173)
(148	28)	(149	16)	(174	10)	(191	14)	(192	34)
(220	34)	(262	41)	(442	38)				

NAME:13C_2179.9_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:218001-11-1

RI:2180

RT:13.638

NUM PEAKS: 57

(72	24)	(73	1000)	(74	88)	(75	135)	(87	30)
(88	12)	(89	32)	(90	20)	(100	15)	(103	27)
(104	190)	(105	22)	(115	8)	(116	13)	(117	13)
(118	28)	(119	72)	(130	8)	(131	27)	(132	50)
(133	55)	(134	19)	(145	27)	(146	21)	(147	222)
(148	40)	(149	57)	(150	7)	(161	13)	(162	24)
(163	12)	(176	23)	(177	10)	(178	52)	(179	5)
(188	9)	(189	8)	(203	26)	(205	7)	(207	42)
(220	78)	(221	22)	(222	9)	(234	7)	(235	18)
(236	6)	(249	9)	(275	4)	(319	5)	(320	6)
(322	8)	(348	7)	(351	10)	(352	34)	(353	9)
(528	8)	(533	3)						

NAME:13C_2217.6_1313EC11_9-(Z)-Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:222001-11-1

RI:2218

RT:13.859

NUM PEAKS: 98

(70	29)	(71	32)	(72	257)	(73	606)	(74	268)
(75	1000)	(76	84)	(77	49)	(83	25)	(84	20)
(85	102)	(86	54)	(87	189)	(88	122)	(89	251)
(90	17)	(91	14)	(93	4)	(96	3)	(97	4)
(98	35)	(99	10)	(100	63)	(101	56)	(102	244)
(103	131)	(104	157)	(105	8)	(106	11)	(113	14)
(114	9)	(115	36)	(116	52)	(117	93)	(118	163)
(119	573)	(120	44)	(121	15)	(128	24)	(130	35)
(131	52)	(132	541)	(133	57)	(134	203)	(135	32)
(136	8)	(143	18)	(144	19)	(145	27)	(146	44)
(148	190)	(149	19)	(150	6)	(158	13)	(159	13)
(160	26)	(161	31)	(162	47)	(163	25)	(164	3)
(173	6)	(174	3)	(176	19)	(177	29)	(178	26)
(179	5)	(180	3)	(188	5)	(190	19)	(191	26)
(192	30)	(193	35)	(194	8)	(205	5)	(206	62)
(208	11)	(221	6)	(222	9)	(223	5)	(236	22)
(237	13)	(238	30)	(250	3)	(251	7)	(252	10)
(253	5)	(266	4)	(268	5)	(281	5)	(282	28)
(283	5)	(284	3)	(355	9)	(356	23)	(357	91)

103

(358 12) (359 5) (372 6)

NAME:13C_2224.7_1313EC11_Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223003-11-1

RI:2225

RT:13.897

NUM PEAKS: 101

(70 36)	(71 36)	(72 267)	(73 936)	(74 286)
(75 1000)	(76 88)	(83 30)	(84 24)	(85 95)
(86 57)	(87 209)	(88 111)	(89 245)	(90 21)
(96 6)	(98 39)	(99 13)	(100 66)	(101 108)
(102 270)	(103 134)	(104 134)	(106 15)	(113 18)
(114 10)	(115 38)	(116 55)	(117 111)	(118 169)
(119 530)	(120 36)	(121 18)	(128 28)	(129 14)
(130 39)	(131 67)	(132 520)	(133 62)	(143 22)
(144 22)	(145 25)	(146 44)	(147 31)	(148 191)
(149 30)	(156 11)	(159 17)	(160 24)	(161 34)
(162 50)	(163 25)	(169 6)	(173 10)	(175 16)
(176 24)	(177 40)	(178 24)	(180 5)	(187 6)
(188 11)	(189 11)	(190 16)	(191 28)	(192 29)
(193 29)	(203 31)	(204 18)	(205 14)	(208 12)
(217 9)	(219 24)	(235 7)	(236 21)	(237 12)
(238 27)	(247 4)	(248 4)	(251 5)	(267 8)
(269 9)	(281 5)	(282 26)	(292 6)	(293 47)
(294 18)	(295 9)	(309 3)	(327 5)	(328 4)
(347 5)	(356 18)	(357 90)	(358 11)	(360 5)
(372 8)	(384 8)	(416 9)	(425 3)	(434 5)
(523 5)				

NAME:13C_2343.5_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:234001-11-1

RI:2344

RT:14.526

NUM PEAKS: 23

(72 22)	(73 1000)	(74 82)	(75 101)	(100 25)
(104 58)	(119 22)	(131 26)	(132 34)	(133 50)
(144 18)	(147 145)	(148 29)	(218 21)	(219 14)
(220 370)	(221 64)	(222 29)	(270 25)	(357 18)
(358 45)	(373 10)	(386 6)		

NAME:13C_2383.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:238002-11-1

RI:2383

RT:14.735

NUM PEAKS: 24

(72 36)	(73 1000)	(74 89)	(75 107)	(89 24)
(90 25)	(103 29)	(104 158)	(118 13)	(119 175)
(131 27)	(132 43)	(133 36)	(147 211)	(148 35)
(149 19)	(161 22)	(162 65)	(163 22)	(173 18)
(191 19)	(206 13)	(207 37)	(220 73)	

NAME:13C_2475.1_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:248002-11-1

RI:2475

RT:15.223

NUM PEAKS: 120

104

(70	16)	(72	29)	(73	1000)	(74	86)	(75	131)
(77	10)	(82	5)	(83	7)	(84	4)	(86	9)
(87	12)	(88	5)	(89	8)	(90	14)	(95	5)
(96	5)	(97	5)	(98	5)	(99	40)	(100	15)
(101	13)	(102	18)	(103	31)	(104	125)	(105	15)
(106	5)	(112	6)	(113	8)	(114	10)	(115	10)
(116	12)	(117	29)	(118	12)	(119	27)	(120	3)
(125	3)	(126	10)	(127	4)	(128	3)	(129	4)
(130	4)	(131	26)	(132	72)	(133	72)	(135	8)
(139	4)	(140	7)	(141	3)	(144	6)	(145	8)
(146	24)	(147	156)	(148	30)	(149	30)	(153	17)
(154	3)	(155	7)	(156	6)	(158	9)	(159	4)
(160	6)	(161	11)	(164	4)	(168	3)	(169	61)
(170	18)	(171	6)	(173	5)	(174	58)	(175	9)
(176	12)	(177	3)	(178	3)	(183	7)	(184	4)
(185	26)	(186	4)	(191	15)	(192	21)	(193	5)
(196	14)	(199	3)	(206	13)	(213	12)	(214	20)
(215	4)	(218	12)	(219	16)	(220	303)	(221	65)
(222	30)	(223	4)	(227	3)	(228	5)	(229	3)
(233	5)	(234	16)	(235	13)	(236	4)	(241	4)
(242	4)	(243	3)	(245	12)	(248	22)	(249	15)
(250	5)	(255	3)	(257	5)	(263	6)	(264	62)
(265	11)	(266	5)	(270	11)	(271	7)	(272	3)
(301	12)	(302	3)	(317	7)	(353	3)	(450	3)

NAME:13C_2732.8_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:273002-11-1

RI:2733

RT:16.587

NUM PEAKS: 64

(71	6)	(72	16)	(73	1000)	(74	89)	(75	85)
(84	5)	(86	25)	(87	11)	(89	31)	(90	16)
(101	11)	(102	8)	(103	27)	(104	123)	(105	36)
(106	8)	(115	10)	(116	9)	(117	9)	(118	13)
(119	76)	(121	5)	(131	21)	(132	90)	(133	56)
(134	21)	(145	6)	(146	23)	(147	259)	(148	46)
(149	27)	(160	15)	(161	16)	(162	83)	(163	20)
(173	8)	(174	52)	(175	8)	(178	8)	(189	5)
(190	10)	(191	25)	(192	34)	(193	9)	(205	9)
(206	244)	(207	107)	(208	26)	(220	122)	(221	32)
(222	11)	(234	7)	(248	44)	(249	12)	(275	3)
(277	23)	(278	9)	(294	6)	(323	18)	(366	22)
(367	132)	(368	40)	(369	18)	(396	4)		

NAME:13C_2814.8_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:281001-11-1

RI:2815

RT:17.009

NUM PEAKS: 53

(72	14)	(73	1000)	(74	83)	(75	81)	(87	9)
(89	25)	(103	40)	(104	74)	(105	20)	(106	6)
(115	10)	(118	18)	(119	52)	(131	22)	(132	81)
(133	56)	(134	20)	(135	7)	(145	10)	(146	18)
(147	273)	(148	47)	(149	30)	(161	17)	(162	67)
(164	30)	(174	37)	(176	6)	(191	32)	(192	42)
(206	264)	(207	106)	(208	28)	(219	9)	(220	80)
(221	176)	(222	45)	(223	20)	(236	6)	(248	19)
(249	11)	(264	7)	(279	6)	(281	30)	(282	9)

105

(295 48) (296 16) (323 9) (324 5) (355 8)
 (367 85) (368 29) (369 34)

NAME:13C_2825.9_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:283001-11-1

RI:2826

RT:17.058

NUM PEAKS: 36

(70 27) (72 174) (73 189) (74 1000) (83 45)
 (86 53) (87 511) (88 20) (89 18) (98 59)
 (100 109) (101 43) (102 144) (104 8) (113 35)
 (114 12) (115 71) (117 59) (128 31) (129 16)
 (130 92) (131 19) (132 58) (143 20) (144 20)
 (145 49) (146 75) (147 59) (158 26) (160 44)
 (171 7) (173 15) (175 8) (203 11) (205 10)
 (218 10)

NAME:13C_2872.6_1313EC11_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-
 D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:287001-11-1

RI:2873

RT:17.266

NUM PEAKS: 58

(73 1000) (74 87) (75 98) (76 9) (86 17)
 (87 12) (88 5) (89 30) (90 12) (101 21)
 (102 13) (103 42) (104 112) (105 28) (115 14)
 (116 13) (118 21) (119 67) (130 7) (131 21)
 (132 115) (133 65) (134 23) (135 9) (145 11)
 (146 21) (147 236) (148 41) (149 27) (160 19)
 (161 26) (162 89) (163 17) (164 25) (173 8)
 (174 61) (175 10) (177 9) (190 6) (191 35)
 (192 49) (205 13) (206 207) (207 59) (208 22)
 (220 115) (234 13) (235 17) (248 29) (249 14)
 (277 23) (278 9) (279 8) (323 16) (366 24)
 (367 140) (368 46) (369 21)

NAME:13C_2907.8_1313EC11_Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-
 (1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:291002-11-1

RI:2908

RT:17.423

NUM PEAKS: 72

(72 14) (73 1000) (74 83) (75 111) (79 18)
 (86 23) (87 14) (89 24) (90 13) (94 12)
 (98 13) (102 23) (103 44) (104 140) (105 26)
 (115 18) (117 12) (118 12) (119 48) (126 10)
 (131 21) (132 93) (133 55) (134 37) (146 26)
 (147 221) (148 40) (160 13) (161 23) (162 74)
 (164 33) (165 15) (174 61) (178 9) (191 26)
 (192 41) (204 12) (206 200) (207 63) (212 9)
 (220 87) (221 19) (233 9) (235 34) (248 31)
 (251 10) (259 8) (262 10) (270 8) (279 14)
 (289 11) (308 20) (309 12) (310 15) (314 9)
 (322 10) (340 12) (366 21) (367 128) (368 43)
 (381 18) (389 14) (397 8) (411 12) (412 7)
 (420 9) (437 17) (448 15) (534 9) (536 10)
 (545 9) (577 6)

106

NAME:13C_2932.1_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:293001-11-1

RI:2932

RT:17.530

NUM PEAKS: 96

(72	14)	(73	1000)	(74	83)	(75	83)	(76	4)
(81	8)	(86	10)	(87	8)	(88	4)	(89	5)
(90	6)	(101	7)	(102	7)	(103	79)	(104	81)
(105	10)	(111	3)	(115	8)	(116	6)	(117	9)
(118	15)	(119	36)	(129	62)	(130	8)	(131	22)
(132	78)	(133	64)	(134	10)	(135	5)	(143	11)
(144	4)	(145	7)	(146	15)	(147	299)	(148	47)
(149	32)	(150	3)	(157	7)	(160	8)	(161	14)
(174	28)	(175	7)	(176	4)	(177	6)	(178	3)
(189	9)	(190	6)	(191	166)	(192	66)	(193	19)
(194	3)	(204	15)	(205	22)	(206	591)	(207	108)
(208	46)	(209	5)	(217	49)	(218	11)	(219	9)
(220	90)	(221	38)	(222	12)	(230	16)	(231	6)
(232	3)	(233	3)	(234	4)	(235	7)	(243	6)
(247	4)	(248	15)	(249	5)	(265	4)	(271	3)
(277	7)	(278	3)	(291	5)	(293	7)	(294	5)
(304	4)	(305	16)	(306	6)	(307	3)	(308	8)
(309	3)	(318	9)	(319	6)	(322	4)	(323	4)
(336	3)	(343	5)	(367	20)	(368	6)	(433	10)
(434	5)								

NAME:13C_2517.7_1313EC11_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:252002-11-1

RI:2518

RT:15.448

NUM PEAKS: 254

(70	14)	(71	36)	(72	107)	(73	1000)	(74	97)
(75	126)	(76	10)	(77	7)	(78	3)	(79	3)
(83	10)	(84	7)	(85	32)	(86	12)	(87	15)
(88	11)	(89	32)	(90	19)	(91	6)	(93	4)
(96	3)	(97	6)	(98	7)	(99	9)	(100	11)
(101	53)	(102	26)	(103	33)	(104	185)	(105	20)
(106	6)	(108	3)	(111	6)	(112	4)	(113	13)
(114	9)	(115	10)	(116	11)	(117	9)	(118	11)
(119	57)	(120	6)	(121	3)	(124	3)	(125	3)
(127	4)	(129	14)	(130	9)	(131	27)	(132	45)
(133	51)	(134	18)	(135	9)	(137	3)	(138	3)
(140	4)	(141	7)	(142	7)	(143	6)	(144	9)
(145	22)	(146	20)	(147	191)	(148	32)	(149	20)
(150	4)	(151	4)	(153	3)	(154	3)	(155	4)
(157	4)	(158	8)	(159	9)	(160	90)	(161	21)
(162	12)	(163	8)	(164	3)	(169	3)	(171	5)
(172	9)	(173	11)	(174	8)	(175	25)	(176	38)
(177	16)	(178	5)	(180	4)	(183	3)	(186	6)
(187	7)	(188	7)	(189	6)	(190	6)	(191	72)
(192	17)	(193	7)	(195	3)	(196	5)	(197	3)
(198	3)	(201	4)	(202	4)	(203	7)	(204	8)
(205	5)	(206	15)	(207	28)	(208	7)	(209	5)
(212	4)	(213	5)	(214	4)	(215	3)	(216	6)
(217	3)	(218	6)	(219	14)	(220	114)	(221	20)
(222	9)	(223	3)	(226	3)	(227	4)	(230	3)
(231	7)	(232	16)	(233	8)	(234	6)	(235	6)

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(236	4)	(239	3)	(244	3)	(245	7)	(246	4)
(247	4)	(248	9)	(249	6)	(250	4)	(253	5)
(257	3)	(260	3)	(261	4)	(262	5)	(263	3)
(264	5)	(265	3)	(266	3)	(267	3)	(268	3)
(274	3)	(276	4)	(277	7)	(278	4)	(279	12)
(280	4)	(289	3)	(293	4)	(294	6)	(295	3)
(296	3)	(301	4)	(302	3)	(304	3)	(305	4)
(306	7)	(307	4)	(308	4)	(309	3)	(310	5)
(313	3)	(319	3)	(320	8)	(321	3)	(322	5)
(323	5)	(324	5)	(325	3)	(326	3)	(333	3)
(334	4)	(335	6)	(336	5)	(337	3)	(338	3)
(339	3)	(341	3)	(344	3)	(347	3)	(349	5)
(350	7)	(351	21)	(352	9)	(353	3)	(361	3)
(363	3)	(364	5)	(365	4)	(367	3)	(368	3)
(372	3)	(376	3)	(377	3)	(380	4)	(381	12)
(382	11)	(383	3)	(387	4)	(388	3)	(394	3)
(395	4)	(396	4)	(397	3)	(409	3)	(412	3)
(422	6)	(423	16)	(424	10)	(425	5)	(427	3)
(437	3)	(439	3)	(442	3)	(447	3)	(449	3)
(450	3)	(452	6)	(453	20)	(454	56)	(455	26)
(456	10)	(457	3)	(460	3)	(467	3)	(470	3)
(480	3)	(481	3)	(491	3)	(492	3)	(503	3)
(506	3)	(508	3)	(513	4)	(514	4)	(515	3)
(516	4)	(519	3)	(522	3)	(526	4)	(535	3)
(536	3)	(542	3)	(544	3)	(569	3)		

NAME:13C_2491.6_1313EC11_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:249001-11-1

RI:2492

RT:15.310

NUM PEAKS: 205

(70	15)	(71	16)	(72	60)	(73	1000)	(74	66)
(75	104)	(77	10)	(82	4)	(85	15)	(86	7)
(87	5)	(88	3)	(89	14)	(90	10)	(92	5)
(93	3)	(96	7)	(98	3)	(99	10)	(100	11)
(101	27)	(102	12)	(103	28)	(104	121)	(105	16)
(106	7)	(108	5)	(110	3)	(111	4)	(113	3)
(114	7)	(115	4)	(116	6)	(117	7)	(118	5)
(119	27)	(123	4)	(126	6)	(128	3)	(129	7)
(131	27)	(132	16)	(133	42)	(134	7)	(139	6)
(141	4)	(142	6)	(143	6)	(144	4)	(145	22)
(146	13)	(147	208)	(148	41)	(149	22)	(150	3)
(151	3)	(155	4)	(158	4)	(159	3)	(160	52)
(161	16)	(162	7)	(163	6)	(168	4)	(169	10)
(170	4)	(171	4)	(172	5)	(173	5)	(174	16)
(175	11)	(176	25)	(177	5)	(185	8)	(186	3)
(188	7)	(189	4)	(191	32)	(192	12)	(193	5)
(194	4)	(195	3)	(196	3)	(202	4)	(203	6)
(204	3)	(205	8)	(206	4)	(207	33)	(208	8)
(210	4)	(211	3)	(213	3)	(214	6)	(216	5)
(218	3)	(219	6)	(220	98)	(221	52)	(222	14)
(223	7)	(231	4)	(232	11)	(233	5)	(234	7)
(235	5)	(236	3)	(237	3)	(239	3)	(245	3)
(248	4)	(249	5)	(252	6)	(256	4)	(257	4)
(258	4)	(261	5)	(263	3)	(264	12)	(265	5)
(266	4)	(267	7)	(270	4)	(273	4)	(274	3)
(275	4)	(276	7)	(277	3)	(279	10)	(280	3)
(281	20)	(282	3)	(283	3)	(288	5)	(295	6)
(309	3)	(310	4)	(317	5)	(319	8)	(320	9)

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(321	3)	(323	5)	(325	8)	(326	3)	(329	3)
(334	3)	(335	3)	(341	7)	(342	4)	(347	3)
(348	4)	(350	5)	(351	19)	(352	7)	(353	3)
(355	18)	(356	9)	(357	4)	(364	3)	(374	4)
(378	4)	(381	12)	(382	6)	(383	3)	(389	3)
(390	3)	(394	4)	(398	3)	(400	3)	(401	4)
(418	3)	(419	3)	(422	5)	(423	12)	(424	6)
(425	4)	(429	5)	(430	6)	(431	5)	(434	3)
(435	5)	(438	3)	(439	4)	(449	5)	(450	4)
(452	7)	(453	19)	(454	53)	(455	20)	(456	8)
(459	4)	(471	4)	(474	5)	(481	6)	(490	4)
(491	5)	(505	4)	(528	3)	(534	3)	(541	3)
(543	3)	(557	3)	(562	4)	(569	3)	(592	3)

NAME:13C_3307.7_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:331001-11-1

RI:3308

RT:19.156

NUM PEAKS: 141

(72	135)	(73	765)	(74	279)	(75	626)	(76	387)
(77	49)	(82	9)	(83	13)	(85	29)	(86	28)
(87	205)	(88	75)	(89	209)	(90	49)	(91	189)
(93	17)	(98	19)	(100	45)	(101	29)	(102	198)
(103	128)	(104	381)	(105	53)	(106	38)	(113	12)
(115	38)	(116	38)	(117	55)	(118	102)	(119	144)
(120	23)	(121	16)	(122	7)	(128	15)	(129	12)
(130	21)	(131	34)	(132	1000)	(133	149)	(134	283)
(135	40)	(136	24)	(141	12)	(142	9)	(145	24)
(147	90)	(148	847)	(149	109)	(150	39)	(156	9)
(157	7)	(158	9)	(160	11)	(161	23)	(162	17)
(163	26)	(164	47)	(165	298)	(171	11)	(175	15)
(177	19)	(178	15)	(179	26)	(183	6)	(189	7)
(192	19)	(193	37)	(194	80)	(195	10)	(207	82)
(208	13)	(209	9)	(211	6)	(220	7)	(221	8)
(222	18)	(224	9)	(229	8)	(230	10)	(232	8)
(234	8)	(237	33)	(238	43)	(239	460)	(240	36)
(241	19)	(242	23)	(244	9)	(248	10)	(250	8)
(252	25)	(253	30)	(254	30)	(255	118)	(256	8)
(267	35)	(282	10)	(285	14)	(289	11)	(291	8)
(299	8)	(308	10)	(309	7)	(311	9)	(312	15)
(313	26)	(314	57)	(315	9)	(325	7)	(328	25)
(329	113)	(330	17)	(331	8)	(332	13)	(334	8)
(343	10)	(344	24)	(345	27)	(357	11)	(358	11)
(375	7)	(381	9)	(391	9)	(392	9)	(402	9)
(403	35)	(404	33)	(408	6)	(428	11)	(461	12)
(493	5)	(497	7)	(498	7)	(501	6)	(508	7)
(511	8)	(523	6)	(569	11)	(570	24)	(571	11)
(573	4)								

NAME:13C_3401.6_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:340002-11-1

RI:3402

RT:19.533

NUM PEAKS: 214

(70	188)	(71	791)	(72	275)	(73	872)	(74	1000)
(75	556)	(76	73)	(77	48)	(80	27)	(81	45)
(82	68)	(83	290)	(84	120)	(85	663)	(86	70)
(87	255)	(88	54)	(89	120)	(91	28)	(95	20)

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(96	56)	(97	193)	(98	289)	(99	243)	(100	230)
(101	48)	(102	278)	(103	49)	(104	32)	(106	7)
(109	9)	(110	34)	(111	108)	(112	70)	(113	399)
(114	43)	(115	196)	(116	27)	(117	179)	(118	11)
(119	48)	(120	16)	(123	13)	(124	73)	(125	75)
(126	120)	(127	124)	(128	191)	(129	35)	(130	133)
(131	55)	(132	358)	(133	43)	(134	36)	(137	35)
(138	70)	(139	100)	(140	67)	(141	228)	(142	55)
(143	167)	(144	87)	(145	429)	(146	76)	(148	18)
(149	12)	(152	54)	(153	46)	(154	103)	(155	92)
(156	151)	(157	85)	(158	143)	(159	43)	(160	100)
(162	31)	(164	23)	(165	17)	(166	21)	(167	42)
(168	48)	(169	114)	(170	36)	(171	129)	(172	38)
(173	114)	(174	29)	(175	57)	(176	9)	(177	23)
(178	15)	(179	13)	(180	16)	(181	17)	(182	30)
(183	38)	(184	57)	(185	34)	(186	99)	(187	38)
(188	94)	(189	21)	(190	37)	(191	9)	(192	14)
(196	20)	(197	53)	(198	12)	(199	58)	(200	49)
(201	107)	(202	30)	(203	47)	(207	17)	(208	10)
(210	10)	(211	28)	(212	24)	(213	16)	(214	42)
(215	12)	(216	56)	(217	19)	(218	41)	(219	26)
(220	46)	(221	11)	(224	12)	(225	19)	(226	12)
(227	15)	(228	11)	(229	33)	(230	16)	(231	26)
(232	11)	(234	13)	(235	34)	(238	9)	(239	17)
(240	13)	(241	8)	(243	8)	(245	10)	(246	20)
(251	12)	(253	14)	(256	14)	(259	63)	(260	10)
(261	46)	(262	18)	(263	19)	(266	14)	(272	8)
(273	10)	(274	24)	(275	18)	(276	29)	(277	51)
(278	22)	(282	10)	(286	10)	(288	11)	(289	11)
(290	9)	(291	12)	(292	16)	(302	14)	(309	10)
(319	14)	(320	9)	(322	10)	(323	8)	(324	8)
(327	10)	(332	11)	(334	10)	(335	13)	(338	14)
(342	12)	(349	16)	(361	7)	(377	11)	(379	12)
(380	15)	(391	9)	(392	12)	(394	10)	(405	11)
(406	13)	(407	43)	(422	13)	(423	25)	(424	12)
(429	15)	(442	6)	(451	11)	(452	9)	(455	7)
(468	13)	(476	11)	(495	7)	(499	9)	(512	24)
(513	45)	(514	13)	(518	8)	(523	6)	(545	10)
(546	9)	(547	8)	(566	8)	(592	6)		

NAME:13C_3494.1_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:349001-11-1

RI:3494

RT:19.905

NUM PEAKS: 70

(70	20)	(72	144)	(73	864)	(74	282)	(75	770)
(76	360)	(77	71)	(86	28)	(87	149)	(88	94)
(89	300)	(90	62)	(91	155)	(92	14)	(93	25)
(100	23)	(101	40)	(102	230)	(103	134)	(104	457)
(105	36)	(106	47)	(116	37)	(117	129)	(118	107)
(119	148)	(120	30)	(122	20)	(130	19)	(131	25)
(132	1000)	(133	166)	(134	281)	(135	29)	(136	22)
(146	21)	(147	65)	(148	858)	(149	130)	(150	20)
(162	23)	(168	12)	(177	35)	(179	15)	(192	26)
(193	51)	(194	114)	(195	217)	(207	78)	(222	17)
(252	15)	(255	43)	(267	38)	(268	49)	(269	376)
(270	30)	(271	16)	(284	13)	(285	45)	(328	26)
(329	140)	(343	21)	(344	73)	(345	40)	(403	32)
(404	43)	(424	12)	(425	12)	(473	10)	(572	9)

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NAME:13C_3334.7_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:334001-11-1

RI:3335

RT:19.264

NUM PEAKS: 191

(70	67)	(71	41)	(72	226)	(73	1000)	(74	566)
(75	796)	(76	188)	(77	53)	(80	29)	(82	43)
(83	123)	(84	46)	(85	184)	(86	56)	(87	294)
(88	66)	(89	119)	(91	57)	(92	23)	(93	24)
(94	21)	(95	33)	(96	37)	(97	46)	(98	274)
(99	40)	(100	189)	(101	54)	(102	240)	(103	57)
(104	89)	(105	16)	(111	39)	(113	267)	(114	31)
(115	147)	(116	53)	(117	137)	(118	34)	(119	51)
(123	25)	(124	120)	(125	33)	(126	138)	(127	75)
(128	328)	(129	63)	(130	137)	(131	43)	(132	156)
(133	59)	(134	156)	(135	21)	(136	20)	(137	82)
(138	184)	(139	182)	(140	57)	(141	209)	(142	70)
(143	142)	(144	47)	(145	84)	(146	45)	(148	118)
(150	22)	(151	40)	(152	155)	(153	144)	(154	364)
(155	109)	(156	333)	(157	62)	(158	100)	(159	24)
(160	57)	(161	21)	(162	20)	(164	56)	(166	63)
(167	148)	(168	80)	(169	268)	(170	141)	(171	212)
(172	49)	(173	77)	(174	33)	(175	60)	(176	16)
(177	19)	(178	51)	(179	28)	(180	46)	(181	49)
(182	126)	(183	58)	(184	158)	(185	58)	(186	88)
(187	31)	(188	32)	(189	29)	(190	16)	(192	24)
(193	38)	(194	19)	(195	55)	(196	37)	(197	106)
(198	48)	(199	126)	(201	45)	(203	29)	(204	23)
(210	50)	(211	46)	(212	105)	(213	60)	(214	108)
(215	23)	(217	17)	(219	42)	(220	19)	(222	27)
(225	23)	(226	31)	(227	128)	(228	43)	(229	54)
(230	29)	(232	15)	(240	23)	(241	24)	(242	53)
(243	50)	(244	65)	(246	24)	(251	17)	(252	15)
(253	12)	(256	15)	(257	16)	(258	15)	(259	35)
(260	18)	(261	30)	(271	24)	(272	58)	(273	15)
(284	17)	(285	26)	(287	19)	(289	11)	(292	13)
(300	17)	(302	18)	(309	22)	(334	15)	(342	9)
(350	16)	(352	14)	(362	38)	(363	83)	(364	112)
(365	15)	(368	14)	(377	20)	(379	16)	(380	14)
(386	20)	(390	28)	(391	108)	(392	163)	(393	42)
(395	13)	(405	22)	(406	16)	(407	33)	(408	33)
(435	14)	(444	17)	(483	21)	(484	15)	(494	14)
(497	32)	(498	35)	(499	13)	(509	17)	(533	13)
(568	8)								

NAME:13C_3347.5_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335001-11-1

RI:3348

RT:19.315

NUM PEAKS: 140

(70	55)	(71	36)	(72	231)	(73	535)	(74	433)
(75	1000)	(76	66)	(77	32)	(82	27)	(83	125)
(84	52)	(85	242)	(86	45)	(87	264)	(88	32)
(89	123)	(90	83)	(96	18)	(97	27)	(98	317)
(99	50)	(100	206)	(101	59)	(102	190)	(103	26)
(104	35)	(111	31)	(112	34)	(113	297)	(114	55)
(115	243)	(116	33)	(117	83)	(123	12)	(124	73)

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(125	24)	(126	123)	(127	39)	(128	179)	(129	44)
(130	85)	(131	30)	(132	64)	(133	12)	(136	10)
(137	29)	(138	73)	(139	100)	(140	37)	(141	180)
(142	51)	(143	131)	(144	45)	(145	64)	(146	17)
(152	53)	(153	47)	(154	108)	(155	50)	(156	173)
(157	58)	(158	117)	(159	19)	(160	54)	(161	55)
(162	18)	(166	21)	(167	39)	(168	21)	(169	88)
(170	42)	(171	145)	(172	29)	(173	70)	(174	24)
(175	25)	(178	8)	(180	11)	(181	18)	(182	35)
(184	66)	(185	18)	(186	70)	(187	23)	(188	24)
(189	17)	(190	26)	(191	8)	(195	8)	(197	26)
(198	15)	(199	63)	(200	27)	(201	39)	(202	13)
(203	31)	(204	24)	(212	34)	(213	19)	(214	43)
(216	36)	(217	27)	(218	15)	(226	13)	(227	51)
(228	27)	(229	112)	(230	14)	(231	15)	(242	21)
(243	28)	(244	78)	(245	27)	(257	16)	(258	14)
(259	11)	(261	12)	(270	6)	(271	21)	(272	86)
(276	7)	(278	7)	(302	25)	(303	9)	(317	16)
(347	20)	(348	11)	(361	46)	(362	210)	(363	44)
(364	14)	(391	15)	(392	29)	(393	18)	(407	20)
(408	51)	(409	13)	(482	17)	(483	9)	(530	8)

NAME:13C_3353.6_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335002-11-1

RT:3354

RT:19.340

NUM PEAKS: 166

(70	62)	(71	62)	(72	175)	(73	888)	(74	215)
(75	1000)	(76	232)	(77	67)	(83	148)	(84	65)
(85	190)	(86	23)	(87	321)	(88	34)	(89	79)
(90	28)	(91	37)	(93	37)	(97	41)	(98	344)
(99	52)	(100	177)	(101	42)	(102	209)	(104	129)
(105	34)	(106	29)	(110	30)	(111	47)	(112	31)
(113	284)	(114	43)	(115	169)	(117	104)	(118	51)
(119	23)	(121	17)	(124	53)	(125	26)	(126	88)
(127	44)	(128	159)	(129	72)	(130	92)	(132	103)
(134	48)	(137	43)	(138	67)	(139	82)	(140	48)
(141	161)	(142	41)	(143	126)	(144	100)	(145	109)
(146	36)	(147	181)	(150	32)	(152	76)	(153	64)
(154	120)	(155	63)	(156	141)	(157	49)	(158	145)
(160	60)	(161	17)	(162	25)	(163	24)	(165	30)
(166	46)	(169	102)	(170	57)	(171	120)	(172	25)
(173	79)	(174	23)	(179	28)	(184	37)	(185	26)
(186	84)	(188	57)	(190	19)	(192	34)	(197	24)
(198	25)	(199	44)	(200	51)	(206	50)	(207	74)
(212	40)	(213	28)	(214	51)	(215	56)	(216	27)
(217	16)	(218	27)	(220	61)	(221	117)	(222	31)
(223	42)	(227	33)	(228	58)	(229	198)	(230	26)
(231	33)	(233	20)	(245	41)	(246	104)	(253	37)
(259	22)	(274	226)	(276	31)	(280	18)	(281	49)
(293	30)	(300	25)	(308	19)	(316	26)	(320	39)
(333	23)	(342	18)	(357	30)	(375	22)	(377	28)
(379	24)	(381	32)	(382	19)	(394	46)	(400	26)
(417	33)	(420	34)	(421	20)	(425	16)	(426	31)
(429	25)	(430	23)	(433	13)	(440	25)	(441	37)
(445	27)	(449	16)	(450	23)	(455	30)	(457	24)
(484	38)	(487	22)	(499	51)	(500	109)	(501	42)
(502	17)	(515	29)	(516	39)	(520	16)	(524	29)
(525	21)	(529	18)	(534	18)	(537	18)	(545	17)

112

(568 12) (569 10) (574 11) (587 11) (590 14)
 (599 7)

NAME:13C_2654.6_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:266001-11-1

RI:2655

RT:16.184

NUM PEAKS: 100

(70 7) (71 12) (72 70) (73 1000) (74 328)
 (75 86) (85 29) (86 16) (87 60) (88 13)
 (89 33) (90 12) (99 8) (100 14) (101 27)
 (102 32) (103 86) (104 312) (105 15) (106 8)
 (114 8) (115 28) (116 13) (118 24) (119 67)
 (120 6) (128 10) (129 7) (130 10) (131 69)
 (132 55) (133 204) (134 8) (143 8) (144 14)
 (145 13) (146 14) (147 210) (148 31) (149 15)
 (157 11) (158 7) (159 20) (160 17) (172 11)
 (173 33) (174 27) (175 30) (176 49) (177 15)
 (187 18) (189 13) (190 28) (191 19) (192 9)
 (202 5) (203 16) (204 23) (205 10) (206 32)
 (207 24) (208 4) (213 11) (216 6) (218 9)
 (219 9) (220 37) (221 8) (224 4) (231 9)
 (232 12) (233 10) (245 5) (246 9) (247 12)
 (273 6) (274 41) (275 22) (276 37) (277 15)
 (294 4) (295 7) (301 4) (302 12) (303 60)
 (304 15) (306 12) (307 61) (308 7) (320 10)
 (334 22) (335 18) (336 42) (337 12) (338 7)
 (393 15) (410 4) (482 6) (483 17) (484 7)

NAME:13C_2689.6_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:269002-11-1

RI:2690

RT:16.369

NUM PEAKS: 259

(70 5) (71 13) (72 10) (73 1000) (74 86)
 (75 48) (76 13) (77 3) (78 3) (82 4)
 (83 3) (84 21) (85 20) (86 47) (87 12)
 (88 13) (90 19) (93 18) (96 7) (97 28)
 (99 20) (100 13) (101 7) (103 42) (104 287)
 (105 56) (108 19) (115 12) (116 4) (117 37)
 (118 18) (119 23) (120 7) (121 4) (127 17)
 (128 4) (130 6) (132 216) (133 51) (134 6)
 (139 7) (140 4) (143 19) (145 9) (146 26)
 (147 259) (148 70) (149 12) (150 20) (151 4)
 (154 7) (156 22) (157 11) (160 66) (161 43)
 (164 8) (168 8) (169 3) (170 9) (171 14)
 (174 187) (175 32) (176 29) (177 34) (178 5)
 (179 8) (182 4) (184 11) (187 9) (188 7)
 (189 6) (190 8) (191 81) (192 427) (193 69)
 (194 17) (199 16) (200 26) (201 11) (204 7)
 (205 38) (206 335) (209 4) (215 8) (216 16)
 (217 12) (220 231) (221 32) (222 10) (231 11)
 (232 9) (233 7) (235 36) (236 13) (238 4)
 (244 19) (246 4) (247 15) (248 66) (249 7)
 (250 5) (251 8) (252 9) (254 6) (255 13)
 (256 7) (257 19) (258 8) (259 4) (260 3)
 (262 12) (263 6) (264 22) (265 7) (266 3)
 (272 5) (274 5) (278 6) (282 21) (285 4)

114

NAME:13C_3185.4_1313EC07_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:318001-11-1
 RI:3185
 RT:18.659

NUM PEAKS: 138

(70	5)	(71	5)	(72	17)	(73	1000)	(74	94)
(75	99)	(76	6)	(77	6)	(84	3)	(85	8)
(86	36)	(87	13)	(88	4)	(89	9)	(90	6)
(98	4)	(100	3)	(101	6)	(102	9)	(103	22)
(104	86)	(105	9)	(106	3)	(114	5)	(115	35)
(116	17)	(117	8)	(118	13)	(119	32)	(130	6)
(131	21)	(132	133)	(133	73)	(134	17)	(135	12)
(137	4)	(144	6)	(145	8)	(146	22)	(147	233)
(148	39)	(149	28)	(151	5)	(158	8)	(159	5)
(160	37)	(161	19)	(162	3)	(173	5)	(174	48)
(175	10)	(176	9)	(177	7)	(178	7)	(181	6)
(186	3)	(187	3)	(188	8)	(189	16)	(190	4)
(191	31)	(192	36)	(193	13)	(195	6)	(203	3)
(204	4)	(205	10)	(206	54)	(207	27)	(208	7)
(209	4)	(210	3)	(211	52)	(212	11)	(213	4)
(218	5)	(219	3)	(220	98)	(221	30)	(222	11)
(225	8)	(227	19)	(232	3)	(233	5)	(234	6)
(235	9)	(236	4)	(243	11)	(245	3)	(246	4)
(247	23)	(248	32)	(249	12)	(250	5)	(255	5)
(261	4)	(262	5)	(275	3)	(276	30)	(277	187)
(278	34)	(279	16)	(283	4)	(285	7)	(294	7)
(298	7)	(299	89)	(300	24)	(301	13)	(308	6)
(309	3)	(313	4)	(314	13)	(315	194)	(316	52)
(317	26)	(318	4)	(322	3)	(323	4)	(338	7)
(359	5)	(366	3)	(367	22)	(368	6)	(373	7)
(386	13)	(387	70)	(388	25)	(389	15)	(390	3)
(428	4)	(429	16)	(430	5)	(431	3)	(518	7)
(519	21)	(520	9)	(521	6)				

NAME:13C_2718.2_1313EC07_
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:272002-11-1
 RI:2718
 RT:16.522

NUM PEAKS: 159

(70	5)	(71	7)	(72	16)	(73	1000)	(74	91)
(75	76)	(76	3)	(77	15)	(79	3)	(84	3)
(85	8)	(86	13)	(87	7)	(88	4)	(89	26)
(90	6)	(91	6)	(98	3)	(99	3)	(100	3)
(101	7)	(102	12)	(103	41)	(104	9)	(105	11)
(106	3)	(107	4)	(114	3)	(115	14)	(116	12)
(117	8)	(118	15)	(119	12)	(121	6)	(129	4)
(130	5)	(131	18)	(132	79)	(133	73)	(134	15)
(135	21)	(136	3)	(137	11)	(144	6)	(145	26)
(146	9)	(147	119)	(148	19)	(149	15)	(150	3)
(151	9)	(158	4)	(159	4)	(160	5)	(161	7)
(163	5)	(165	4)	(167	3)	(173	5)	(174	5)
(175	4)	(176	28)	(177	6)	(179	3)	(181	13)
(182	3)	(183	5)	(186	8)	(187	4)	(188	3)
(189	4)	(190	3)	(191	14)	(192	16)	(193	16)
(194	4)	(195	14)	(196	3)	(197	4)	(202	6)
(203	4)	(204	3)	(205	4)	(206	24)	(207	23)
(208	6)	(209	6)	(210	3)	(211	74)	(212	12)
(213	7)	(218	4)	(219	5)	(220	88)	(221	18)

115

(222	8)	(225	30)	(226	7)	(227	19)	(228	3)
(233	4)	(234	5)	(237	9)	(238	3)	(241	3)
(242	4)	(243	4)	(248	3)	(255	5)	(268	3)
(269	3)	(274	5)	(275	3)	(276	4)	(283	7)
(284	4)	(285	8)	(298	17)	(299	157)	(300	47)
(301	24)	(302	5)	(306	3)	(313	4)	(314	19)
(315	153)	(316	44)	(317	23)	(318	4)	(329	4)
(343	6)	(355	3)	(356	14)	(357	7)	(358	8)
(359	25)	(360	8)	(361	4)	(371	3)	(372	5)
(373	6)	(374	3)	(385	4)	(386	28)	(387	100)
(388	41)	(389	22)	(390	5)	(416	6)	(417	16)
(418	6)	(419	3)	(450	3)	(451	6)	(452	3)
(461	4)	(462	12)	(463	6)	(464	3)		

NAME:13C_2724.4_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:272001-11-1

RI:2724

RT:16.554

NUM PEAKS: 143

(70	6)	(71	6)	(72	17)	(73	1000)	(74	92)
(75	75)	(76	4)	(77	15)	(85	9)	(86	11)
(87	6)	(88	3)	(89	36)	(90	7)	(91	7)
(98	3)	(99	3)	(100	3)	(101	8)	(102	12)
(103	44)	(104	15)	(105	13)	(106	3)	(107	5)
(114	3)	(115	14)	(116	10)	(117	9)	(118	14)
(119	13)	(120	3)	(121	6)	(123	3)	(129	4)
(130	5)	(131	18)	(132	94)	(133	74)	(134	17)
(135	22)	(136	3)	(137	12)	(144	5)	(145	30)
(146	9)	(147	109)	(148	17)	(149	14)	(151	10)
(158	3)	(159	4)	(160	4)	(161	8)	(163	6)
(165	4)	(167	3)	(173	4)	(175	4)	(176	34)
(177	7)	(179	3)	(181	14)	(182	3)	(183	4)
(186	4)	(189	4)	(190	3)	(191	12)	(193	13)
(194	3)	(195	15)	(196	3)	(197	4)	(202	4)
(203	3)	(205	4)	(207	24)	(208	6)	(209	6)
(210	4)	(211	71)	(212	11)	(213	7)	(218	4)
(219	6)	(220	91)	(221	17)	(222	8)	(225	39)
(226	8)	(227	18)	(228	3)	(233	3)	(234	6)
(237	10)	(238	3)	(241	4)	(242	4)	(243	3)
(255	4)	(268	4)	(269	4)	(274	4)	(277	3)
(283	8)	(284	4)	(285	8)	(298	18)	(299	171)
(300	50)	(301	25)	(302	5)	(313	5)	(314	18)
(315	149)	(316	42)	(317	22)	(318	4)	(329	4)
(343	6)	(355	3)	(356	11)	(357	6)	(358	8)
(359	25)	(360	8)	(361	4)	(372	3)	(373	6)
(374	3)	(385	5)	(386	34)	(387	121)	(388	49)
(389	26)	(390	7)	(417	5)	(451	5)	(461	3)
(462	9)	(463	4)	(550	3)				

NAME:13C_2562.2_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:256001-11-1

RI:2562

RT:15.693

NUM PEAKS: 136

(71	8)	(72	18)	(73	1000)	(74	92)	(75	88)
(76	8)	(77	10)	(84	3)	(85	21)	(86	7)
(87	9)	(88	5)	(89	39)	(90	13)	(91	6)
(98	3)	(100	4)	(101	9)	(102	12)	(103	40)

116

(104	98)	(105	20)	(106	6)	(107	3)	(114	3)
(115	10)	(116	18)	(117	9)	(118	15)	(119	24)
(120	5)	(121	5)	(129	3)	(130	5)	(131	20)
(132	72)	(133	62)	(134	30)	(135	16)	(136	3)
(137	5)	(144	3)	(145	10)	(146	11)	(147	133)
(148	24)	(150	5)	(151	5)	(158	4)	(160	6)
(161	29)	(162	6)	(163	6)	(164	3)	(165	3)
(173	11)	(174	7)	(175	4)	(176	12)	(177	5)
(181	6)	(183	3)	(188	3)	(189	4)	(190	3)
(191	15)	(192	15)	(193	10)	(194	3)	(195	6)
(203	5)	(204	5)	(205	4)	(206	25)	(207	17)
(208	5)	(209	3)	(211	37)	(212	6)	(213	3)
(218	4)	(219	6)	(220	38)	(221	9)	(222	6)
(225	11)	(227	8)	(232	4)	(233	4)	(234	3)
(235	4)	(243	3)	(247	3)	(248	3)	(249	3)
(250	3)	(251	6)	(255	5)	(264	5)	(265	10)
(266	5)	(283	5)	(284	3)	(285	5)	(298	10)
(299	89)	(300	28)	(301	12)	(313	3)	(314	7)
(315	41)	(316	12)	(317	6)	(329	4)	(331	3)
(336	4)	(343	6)	(344	3)	(358	8)	(359	34)
(360	11)	(361	5)	(372	3)	(373	4)	(385	4)
(386	33)	(387	116)	(388	51)	(389	24)	(390	6)
(403	3)	(474	6)	(475	16)	(476	8)	(477	5)
(478	3)								

NAME:13C 2579.9 1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:258001-11-1

RI:2580

RT:15.787

NUM PEAKS: 335

(70	29)	(71	30)	(72	214)	(73	1000)	(74	332)
(75	309)	(76	39)	(77	31)	(78	6)	(79	8)
(80	6)	(82	7)	(83	27)	(84	13)	(85	68)
(86	31)	(87	155)	(88	55)	(89	137)	(90	45)
(91	15)	(92	8)	(93	7)	(94	6)	(96	7)
(98	32)	(99	11)	(100	49)	(101	31)	(102	121)
(103	171)	(104	352)	(105	49)	(106	19)	(109	6)
(111	8)	(113	11)	(114	8)	(115	36)	(116	22)
(117	59)	(118	109)	(119	135)	(120	22)	(121	6)
(122	5)	(124	6)	(125	7)	(126	3)	(128	15)
(129	12)	(130	49)	(131	51)	(132	492)	(133	179)
(134	136)	(135	31)	(136	5)	(137	4)	(138	7)
(139	7)	(141	7)	(142	6)	(143	13)	(144	12)
(145	41)	(146	19)	(147	420)	(148	106)	(149	73)
(150	24)	(151	10)	(152	7)	(153	6)	(154	3)
(156	10)	(157	6)	(158	11)	(159	10)	(160	24)
(161	17)	(162	16)	(163	15)	(164	9)	(165	8)
(167	5)	(168	6)	(169	5)	(170	5)	(171	4)
(172	8)	(173	8)	(174	6)	(175	11)	(176	8)
(177	24)	(178	13)	(179	6)	(180	3)	(181	4)
(183	5)	(184	3)	(185	4)	(186	4)	(187	6)
(188	6)	(190	8)	(191	9)	(192	22)	(193	16)
(194	6)	(195	6)	(196	6)	(197	4)	(198	5)
(199	4)	(200	3)	(201	3)	(202	8)	(203	4)
(204	3)	(205	9)	(206	147)	(207	139)	(208	29)
(209	13)	(210	5)	(221	9)	(222	35)	(223	9)
(224	11)	(226	7)	(229	5)	(231	4)	(232	3)
(233	3)	(234	12)	(235	15)	(236	5)	(237	7)
(238	7)	(239	5)	(240	11)	(241	6)	(242	7)

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(243	4)	(244	3)	(245	4)	(246	8)	(247	4)
(249	4)	(250	4)	(252	20)	(253	43)	(254	8)
(256	4)	(260	4)	(262	4)	(265	5)	(266	7)
(267	31)	(268	15)	(269	7)	(270	5)	(271	4)
(272	4)	(275	3)	(279	6)	(280	9)	(281	5)
(282	8)	(283	6)	(284	3)	(285	4)	(290	3)
(292	7)	(294	4)	(295	4)	(296	8)	(297	24)
(298	11)	(300	5)	(301	4)	(302	4)	(303	3)
(305	4)	(306	5)	(307	3)	(309	9)	(310	7)
(311	7)	(312	6)	(313	3)	(314	6)	(315	5)
(316	8)	(317	5)	(318	4)	(319	3)	(320	4)
(321	3)	(322	5)	(325	11)	(326	10)	(327	14)
(328	3)	(329	4)	(331	7)	(332	6)	(334	5)
(337	5)	(338	4)	(340	7)	(344	6)	(345	6)
(347	5)	(348	6)	(353	3)	(355	8)	(356	6)
(357	5)	(360	4)	(361	7)	(371	6)	(373	5)
(374	4)	(375	5)	(378	4)	(381	7)	(382	5)
(383	4)	(384	5)	(385	15)	(386	27)	(387	88)
(388	29)	(389	9)	(390	4)	(391	4)	(395	6)
(396	6)	(397	4)	(398	7)	(399	7)	(400	8)
(401	15)	(402	7)	(403	10)	(406	4)	(408	4)
(409	3)	(410	5)	(412	4)	(415	7)	(419	5)
(420	5)	(422	3)	(423	5)	(424	5)	(429	4)
(430	3)	(431	7)	(432	4)	(438	4)	(439	6)
(440	4)	(441	3)	(443	4)	(444	4)	(446	4)
(447	4)	(453	3)	(454	4)	(455	5)	(456	5)
(458	5)	(459	6)	(460	4)	(461	4)	(462	5)
(463	5)	(464	6)	(465	5)	(466	3)	(467	3)
(472	5)	(473	6)	(474	4)	(475	9)	(476	12)
(477	9)	(478	6)	(479	4)	(483	4)	(484	4)
(485	6)	(486	4)	(488	5)	(491	4)	(492	6)
(493	6)	(496	3)	(497	4)	(502	4)	(503	5)
(506	5)	(508	3)	(509	5)	(512	4)	(517	3)
(522	7)	(525	4)	(526	4)	(528	5)	(531	4)
(536	3)	(539	3)	(540	3)	(541	7)	(542	3)
(544	5)	(546	4)	(547	4)	(548	3)	(550	3)
(551	3)	(552	4)	(555	3)	(558	5)	(561	4)
(564	3)	(572	4)	(584	3)	(590	3)	(591	3)

NAME:13C 2390.1_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:239001-11-1

RI:2390

RT:14.779

NUM PEAKS: 108

(70	5)	(71	9)	(73	1000)	(74	90)	(75	102)
(76	7)	(77	11)	(84	3)	(85	8)	(86	16)
(87	8)	(88	4)	(89	7)	(90	4)	(99	3)
(100	3)	(101	5)	(102	9)	(103	28)	(104	29)
(105	10)	(107	3)	(113	3)	(114	5)	(115	15)
(116	15)	(117	8)	(118	14)	(119	15)	(121	3)
(130	4)	(131	22)	(132	113)	(133	65)	(134	13)
(135	15)	(137	5)	(145	5)	(146	13)	(147	149)
(148	26)	(149	22)	(150	3)	(151	5)	(160	10)
(161	7)	(164	3)	(174	10)	(175	3)	(176	3)
(177	3)	(181	6)	(189	5)	(191	26)	(192	37)
(193	16)	(194	4)	(195	6)	(205	7)	(206	163)
(207	40)	(208	15)	(209	3)	(211	41)	(212	7)
(213	4)	(219	3)	(220	45)	(221	11)	(222	5)
(225	9)	(226	3)	(227	8)	(235	3)	(243	3)

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(247	5)	(248	6)	(249	3)	(255	5)	(271	4)
(276	6)	(277	13)	(278	3)	(283	4)	(285	5)
(298	11)	(299	98)	(300	28)	(301	13)	(302	3)
(308	4)	(314	6)	(315	28)	(316	8)	(317	4)
(351	6)	(358	6)	(359	26)	(360	8)	(361	4)
(372	5)	(373	17)	(374	6)	(386	24)	(387	82)
(388	35)	(389	18)	(390	5)				

NAME:13C_2347.2_1313EC07_Glucose-6-phosphate methoxyamine (BP) (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:235002-11-1

RI:2347

RT:14.551

NUM PEAKS: 96

(70	5)	(71	10)	(72	16)	(73	1000)	(74	89)
(75	79)	(76	5)	(85	8)	(86	5)	(87	8)
(88	3)	(89	49)	(90	9)	(101	13)	(102	12)
(104	43)	(107	3)	(115	8)	(116	11)	(118	17)
(119	12)	(120	3)	(121	4)	(131	17)	(132	73)
(133	70)	(134	18)	(135	15)	(137	6)	(145	4)
(146	9)	(147	114)	(148	19)	(149	13)	(151	6)
(158	3)	(160	4)	(161	33)	(162	40)	(163	15)
(164	3)	(173	3)	(174	5)	(181	7)	(192	7)
(193	10)	(194	3)	(195	8)	(197	3)	(207	15)
(208	3)	(209	3)	(211	46)	(212	8)	(213	4)
(220	30)	(225	13)	(226	3)	(227	10)	(233	4)
(234	5)	(235	5)	(243	4)	(248	3)	(251	6)
(255	5)	(283	4)	(285	4)	(298	12)	(299	105)
(300	32)	(301	15)	(302	3)	(313	3)	(314	8)
(315	46)	(316	14)	(317	7)	(331	4)	(343	5)
(344	3)	(358	8)	(359	35)	(360	11)	(361	5)
(373	4)	(385	3)	(386	32)	(387	116)	(388	49)
(389	26)	(390	7)	(474	4)	(475	12)	(476	6)
(477	3)								

NAME:13C_2313.4_1313EC07_Galactose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232001-11-1

RI:2313

RT:14.372

NUM PEAKS: 108

(70	5)	(71	5)	(72	17)	(73	1000)	(74	90)
(75	91)	(76	5)	(77	9)	(86	9)	(87	11)
(88	5)	(89	37)	(90	8)	(91	4)	(100	3)
(101	14)	(102	12)	(103	48)	(105	23)	(106	4)
(107	3)	(115	10)	(116	17)	(117	9)	(118	16)
(119	14)	(121	4)	(129	3)	(130	6)	(131	20)
(132	72)	(133	66)	(134	16)	(135	15)	(137	6)
(144	4)	(145	7)	(146	11)	(147	144)	(148	24)
(149	16)	(151	6)	(159	3)	(160	5)	(161	30)
(162	61)	(163	14)	(164	4)	(173	4)	(174	5)
(175	3)	(176	5)	(177	4)	(181	7)	(189	3)
(190	3)	(191	14)	(192	9)	(193	11)	(195	8)
(203	3)	(204	3)	(205	4)	(206	12)	(207	19)
(208	5)	(209	3)	(211	42)	(212	7)	(213	4)
(218	6)	(219	8)	(225	12)	(226	3)	(227	10)
(232	3)	(233	4)	(234	6)	(235	5)	(248	3)
(249	3)	(251	4)	(255	5)	(283	4)	(285	4)
(298	9)	(299	89)	(300	26)	(301	13)	(302	3)
(331	6)	(336	6)	(343	6)	(358	7)	(359	32)

119

(360 10) (361 5) (373 3) (385 3) (386 27)
 (387 101) (388 42) (389 23) (390 6) (474 4)
 (475 11) (476 5) (477 3)

NAME:13C_2311.9_1313EC07_Fructose-6-phosphate methoxyamine (6TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:232002-11-1

RI:2312

RT:14.363

NUM PEAKS: 135

(70 4) (71 8) (72 12) (73 1000) (74 93)
 (75 16) (77 5) (85 27) (86 5) (89 36)
 (90 15) (91 6) (98 3) (101 4) (102 5)
 (103 37) (104 122) (105 12) (106 7) (114 3)
 (115 7) (116 18) (117 8) (118 12) (119 33)
 (120 7) (129 4) (130 4) (131 19) (132 87)
 (133 47) (134 30) (135 14) (137 6) (142 3)
 (145 9) (146 5) (147 163) (148 27) (149 18)
 (150 3) (151 5) (158 3) (159 4) (160 6)
 (173 9) (174 3) (175 3) (176 7) (177 3)
 (181 8) (183 3) (186 4) (188 3) (189 4)
 (191 6) (192 11) (193 9) (195 8) (203 4)
 (204 3) (205 3) (206 14) (207 16) (208 6)
 (209 3) (211 52) (212 10) (213 5) (217 3)
 (218 3) (219 9) (220 177) (221 39) (222 17)
 (223 4) (225 15) (226 4) (227 21) (228 4)
 (233 3) (237 3) (248 4) (249 3) (255 5)
 (260 3) (261 4) (262 3) (263 3) (264 5)
 (265 10) (266 4) (267 3) (274 3) (276 3)
 (283 3) (285 5) (297 3) (298 10) (299 86)
 (300 31) (301 15) (302 4) (306 3) (307 3)
 (308 3) (309 3) (313 3) (314 28) (315 274)
 (316 79) (317 41) (318 8) (319 3) (322 3)
 (323 3) (329 4) (343 6) (344 3) (345 3)
 (358 5) (359 19) (360 7) (361 4) (362 3)
 (372 3) (373 7) (374 5) (402 4) (403 11)
 (404 5) (461 12) (462 30) (463 14) (464 6)

NAME:13C_2257.9_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:226001-11-1

RI:2258

RT:14.076

NUM PEAKS: 138

(70 7) (71 10) (72 31) (73 1000) (74 113)
 (75 105) (76 8) (84 5) (85 15) (86 9)
 (87 25) (88 20) (89 245) (90 21) (98 3)
 (99 3) (100 9) (101 16) (102 13) (103 20)
 (104 187) (105 17) (106 5) (113 4) (114 5)
 (115 9) (116 12) (118 12) (119 53) (130 8)
 (131 25) (132 24) (133 39) (134 10) (142 4)
 (144 6) (145 19) (146 20) (147 228) (148 44)
 (149 22) (156 3) (157 5) (158 4) (159 7)
 (160 8) (161 10) (163 5) (171 3) (172 6)
 (173 14) (174 5) (175 8) (176 12) (177 7)
 (178 5) (179 26) (180 3) (186 5) (187 6)
 (188 9) (189 7) (190 3) (191 19) (192 16)
 (193 7) (202 4) (203 5) (204 6) (205 5)
 (207 25) (208 28) (209 4) (214 3) (218 3)
 (219 7) (220 78) (221 20) (222 6) (232 4)

120

(233	12)	(246	3)	(247	8)	(248	3)	(251	3)
(259	3)	(260	4)	(261	7)	(262	6)	(263	4)
(265	6)	(266	3)	(274	3)	(275	4)	(276	6)
(277	3)	(278	3)	(279	7)	(280	3)	(291	3)
(292	3)	(293	3)	(294	4)	(296	3)	(304	3)
(305	3)	(306	3)	(307	4)	(309	3)	(310	7)
(334	5)	(335	14)	(336	7)	(337	3)	(350	3)
(351	6)	(352	5)	(378	4)	(379	3)	(380	8)
(381	9)	(382	23)	(383	7)	(410	3)	(411	4)
(441	3)	(442	4)	(452	3)	(453	8)	(454	4)
(468	4)	(483	4)	(484	3)	(558	5)	(559	3)
(560	3)	(561	6)	(562	3)				

NAME:13C_2294.1_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:230001-11-1

RI:2294

RT:14.269

NUM PEAKS: 188

(70	7)	(71	5)	(73	758)	(74	78)	(75	66)
(80	4)	(82	5)	(86	7)	(90	24)	(94	9)
(97	6)	(99	15)	(103	62)	(104	320)	(105	34)
(107	9)	(110	12)	(112	9)	(113	4)	(115	21)
(116	18)	(117	21)	(118	21)	(125	5)	(130	14)
(132	78)	(133	56)	(135	12)	(136	7)	(141	5)
(143	11)	(144	8)	(146	31)	(148	24)	(149	20)
(152	7)	(153	5)	(156	8)	(157	24)	(161	11)
(162	11)	(164	12)	(166	8)	(168	13)	(172	7)
(173	6)	(174	15)	(176	7)	(179	12)	(183	6)
(184	9)	(185	9)	(187	11)	(188	6)	(191	31)
(192	54)	(193	9)	(195	14)	(196	6)	(197	9)
(198	8)	(199	8)	(200	9)	(204	8)	(205	40)
(206	1000)	(207	122)	(208	63)	(213	6)	(214	6)
(215	12)	(217	22)	(218	7)	(220	50)	(221	23)
(222	41)	(223	8)	(232	6)	(234	9)	(236	15)
(237	15)	(243	7)	(244	13)	(246	5)	(247	7)
(252	7)	(253	8)	(257	6)	(259	12)	(260	15)
(263	14)	(264	10)	(268	12)	(269	16)	(271	10)
(272	17)	(278	6)	(292	10)	(302	6)	(308	7)
(309	7)	(317	14)	(323	10)	(324	10)	(326	10)
(330	7)	(332	12)	(333	6)	(339	15)	(340	15)
(341	39)	(343	12)	(345	9)	(346	8)	(353	12)
(364	14)	(365	13)	(366	12)	(367	20)	(368	9)
(371	12)	(376	14)	(378	12)	(379	13)	(383	13)
(384	10)	(389	9)	(390	5)	(391	12)	(394	8)
(395	8)	(402	18)	(408	9)	(410	10)	(411	7)
(415	7)	(421	13)	(426	8)	(430	10)	(443	13)
(447	24)	(448	9)	(449	10)	(453	16)	(454	12)
(458	9)	(459	12)	(461	11)	(471	8)	(477	9)
(480	18)	(483	6)	(484	13)	(488	10)	(489	8)
(491	9)	(493	13)	(494	8)	(499	12)	(502	10)
(503	15)	(504	7)	(505	8)	(509	12)	(510	12)
(513	18)	(514	14)	(515	17)	(524	8)	(528	12)
(529	9)	(532	8)	(533	13)	(548	14)	(549	16)
(553	7)	(555	16)	(559	5)	(560	6)	(563	7)
(566	7)	(569	12)	(571	13)	(575	7)	(578	4)
(580	6)	(590	7)	(591	8)				

NAME:13C_2285.3_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:228001-11-1

RI:2285

RT:14.222

NUM PEAKS: 106

(71	7)	(72	20)	(73	1000)	(74	95)	(75	145)
(76	9)	(77	5)	(85	6)	(86	9)	(87	12)
(88	4)	(89	39)	(90	15)	(100	4)	(101	17)
(102	15)	(103	51)	(104	36)	(105	26)	(106	3)
(116	14)	(117	10)	(118	133)	(119	330)	(120	29)
(121	13)	(130	5)	(131	16)	(132	62)	(133	44)
(134	15)	(135	5)	(144	4)	(145	9)	(146	25)
(147	132)	(148	25)	(149	18)	(160	8)	(161	98)
(162	120)	(163	60)	(164	10)	(165	3)	(173	5)
(174	5)	(176	6)	(177	6)	(190	3)	(191	16)
(192	9)	(193	11)	(203	3)	(204	4)	(206	6)
(207	9)	(209	4)	(215	3)	(216	5)	(218	6)
(219	10)	(220	71)	(221	20)	(222	9)	(233	4)
(234	8)	(235	16)	(236	7)	(237	15)	(238	3)
(248	5)	(251	13)	(252	3)	(253	13)	(262	5)
(263	3)	(264	3)	(265	4)	(274	3)	(278	4)
(280	5)	(281	4)	(294	4)	(296	10)	(297	82)
(298	16)	(306	4)	(307	3)	(308	4)	(309	3)
(310	4)	(323	10)	(324	4)	(325	10)	(326	3)
(327	3)	(333	3)	(334	4)	(352	3)	(368	3)
(412	6)	(413	25)	(414	9)	(415	4)	(441	3)
(513	3)								

NAME:13C_1396.1_1313EC11

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140003-11-1

RI:1396

RT: 7.541

NUM PEAKS: 66

(70	5)	(71	5)	(72	21)	(73	1000)	(74	85)
(75	322)	(76	10)	(77	10)	(84	1)	(85	6)
(86	2)	(91	12)	(99	2)	(103	50)	(104	8)
(105	6)	(110	1)	(112	3)	(117	13)	(118	192)
(119	660)	(120	59)	(121	21)	(126	2)	(133	129)
(134	15)	(135	14)	(136	2)	(137	2)	(144	3)
(146	9)	(149	115)	(150	15)	(161	2)	(163	4)
(176	9)	(177	11)	(178	4)	(191	2)	(192	2)
(193	3)	(200	4)	(207	13)	(208	3)	(209	2)
(211	1)	(216	2)	(235	3)	(236	10)	(237	134)
(238	23)	(239	9)	(242	1)	(249	1)	(250	24)
(251	3)	(252	3)	(268	6)	(288	1)	(308	7)
(309	89)	(310	24)	(311	14)	(312	2)	(340	7)
(341	2)								

NAME:13C_1475.5_1313EC07_Citramalic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148001-11-1

RI:1476

RT: 8.482

NUM PEAKS: 94

(70	7)	(71	15)	(72	90)	(73	1000)	(74	95)
(75	209)	(76	21)	(77	7)	(86	3)	(87	10)
(88	5)	(89	37)	(100	11)	(101	9)	(102	18)
(103	14)	(104	5)	(116	5)	(117	16)	(118	125)
(119	15)	(120	4)	(131	28)	(132	10)	(133	76)
(134	11)	(135	10)	(136	1)	(137	1)	(146	9)

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(147	368)	(148	69)	(149	76)	(150	10)	(151	7)
(152	1)	(160	4)	(161	19)	(162	2)	(163	28)
(164	4)	(165	2)	(174	4)	(175	5)	(176	3)
(178	1)	(190	22)	(191	9)	(192	21)	(193	8)
(194	2)	(206	31)	(207	11)	(208	3)	(211	2)
(218	1)	(219	8)	(221	32)	(222	7)	(223	3)
(224	1)	(227	2)	(229	1)	(234	26)	(235	35)
(236	18)	(237	5)	(238	1)	(247	1)	(250	7)
(251	136)	(252	23)	(253	11)	(254	1)	(263	2)
(264	32)	(265	5)	(266	4)	(280	3)	(293	1)
(299	3)	(301	1)	(308	2)	(309	4)	(310	1)
(322	1)	(324	1)	(325	15)	(326	6)	(337	2)
(338	1)	(353	1)	(354	10)	(355	3)		

NAME:13C 1735.8 1313EC07_Glycerol-2-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174002-11-1

RI:1736

RT: 10.586

NUM PEAKS: 421

(70	8)	(71	21)	(72	39)	(73	1000)	(74	110)
(75	219)	(76	14)	(77	39)	(78	3)	(79	13)
(80	14)	(81	10)	(82	19)	(83	10)	(84	26)
(85	11)	(86	1)	(87	155)	(88	35)	(89	31)
(90	8)	(91	27)	(92	8)	(93	5)	(94	7)
(95	3)	(96	4)	(98	16)	(99	11)	(100	28)
(101	25)	(102	49)	(103	149)	(105	26)	(106	11)
(107	16)	(108	3)	(109	10)	(111	10)	(112	10)
(113	14)	(114	6)	(115	51)	(116	20)	(117	29)
(118	82)	(121	25)	(124	15)	(127	24)	(128	34)
(129	33)	(130	24)	(131	47)	(132	136)	(133	81)
(134	15)	(135	20)	(136	5)	(137	14)	(138	8)
(139	6)	(141	49)	(142	12)	(144	12)	(146	15)
(147	185)	(148	5)	(149	12)	(151	24)	(152	34)
(153	19)	(154	4)	(155	27)	(156	19)	(157	61)
(158	2)	(159	23)	(160	11)	(162	13)	(165	4)
(166	10)	(167	2)	(168	2)	(169	2)	(170	9)
(171	7)	(172	7)	(174	1)	(175	435)	(176	28)
(177	42)	(178	5)	(179	22)	(180	95)	(181	46)
(182	16)	(183	16)	(184	15)	(185	15)	(186	19)
(187	4)	(189	25)	(190	73)	(191	3)	(192	14)
(193	23)	(194	8)	(195	12)	(196	14)	(197	18)
(198	29)	(199	8)	(201	15)	(202	5)	(203	25)
(205	1)	(210	3)	(211	227)	(212	41)	(213	31)
(214	9)	(215	6)	(216	9)	(217	18)	(218	21)
(223	14)	(224	3)	(225	8)	(227	38)	(228	2)
(229	13)	(230	1)	(231	76)	(232	24)	(234	2)
(235	2)	(236	5)	(238	14)	(239	4)	(240	6)
(242	20)	(243	294)	(244	54)	(245	38)	(246	11)
(247	3)	(249	11)	(251	1)	(252	9)	(253	9)
(255	7)	(256	6)	(257	9)	(258	3)	(259	17)
(260	16)	(261	8)	(263	5)	(265	10)	(266	3)
(267	9)	(268	14)	(269	83)	(270	22)	(271	8)
(272	3)	(273	3)	(274	12)	(275	14)	(276	12)
(277	13)	(280	9)	(282	6)	(283	26)	(284	17)
(285	32)	(286	12)	(287	12)	(288	6)	(291	4)
(294	8)	(295	8)	(296	7)	(297	5)	(298	19)
(299	173)	(300	60)	(301	36)	(302	8)	(303	5)
(304	6)	(306	1)	(308	32)	(309	24)	(311	3)
(312	7)	(313	9)	(314	14)	(315	36)	(316	14)

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(318	7)	(319	6)	(320	9)	(321	25)	(322	4)
(326	8)	(329	12)	(330	3)	(331	12)	(332	9)
(333	8)	(334	7)	(337	9)	(338	9)	(339	9)
(340	9)	(341	4)	(343	8)	(344	2)	(345	5)
(346	9)	(347	12)	(348	22)	(349	8)	(351	13)
(352	9)	(353	8)	(355	8)	(356	7)	(357	9)
(358	5)	(359	8)	(360	10)	(361	5)	(362	5)
(363	12)	(364	3)	(365	4)	(370	11)	(371	3)
(372	13)	(373	21)	(374	15)	(375	21)	(376	13)
(377	12)	(378	18)	(379	3)	(380	15)	(381	5)
(384	5)	(385	15)	(386	7)	(387	6)	(388	7)
(389	27)	(390	18)	(391	4)	(392	10)	(393	9)
(394	10)	(395	9)	(396	12)	(397	6)	(398	3)
(399	14)	(400	9)	(401	17)	(402	1)	(403	6)
(404	13)	(405	6)	(407	7)	(408	3)	(409	4)
(411	12)	(414	2)	(415	7)	(416	15)	(417	11)
(418	8)	(419	4)	(420	7)	(421	2)	(422	3)
(423	15)	(424	4)	(426	13)	(427	2)	(429	5)
(430	2)	(431	1)	(432	4)	(433	1)	(435	3)
(436	15)	(437	7)	(439	13)	(440	15)	(441	1)
(442	5)	(443	2)	(444	3)	(446	6)	(447	6)
(448	22)	(449	12)	(450	5)	(451	6)	(452	7)
(453	4)	(454	10)	(455	12)	(457	2)	(459	12)
(460	12)	(461	11)	(463	10)	(466	6)	(467	9)
(470	15)	(471	12)	(472	3)	(473	9)	(475	14)
(476	10)	(478	1)	(479	6)	(480	10)	(481	6)
(482	8)	(483	1)	(484	9)	(485	13)	(486	2)
(487	5)	(488	6)	(489	4)	(491	10)	(492	6)
(493	10)	(494	8)	(495	9)	(496	5)	(498	8)
(499	9)	(500	6)	(501	8)	(502	2)	(503	7)
(504	9)	(505	2)	(507	9)	(508	5)	(509	23)
(510	9)	(512	7)	(513	3)	(514	2)	(516	11)
(517	9)	(518	7)	(519	8)	(520	6)	(521	5)
(522	11)	(523	2)	(524	10)	(525	9)	(527	5)
(528	18)	(529	13)	(530	15)	(531	3)	(532	4)
(534	2)	(535	11)	(536	6)	(538	5)	(539	2)
(540	5)	(541	3)	(542	6)	(543	12)	(544	6)
(546	5)	(550	11)	(551	8)	(552	11)	(554	3)
(555	4)	(557	1)	(558	9)	(561	10)	(562	4)
(563	6)	(564	1)	(565	7)	(566	9)	(569	1)
(570	3)	(571	2)	(572	11)	(573	9)	(574	3)
(575	1)	(576	1)	(578	2)	(581	3)	(582	1)
(583	2)	(584	9)	(587	1)	(588	8)	(590	1)
(591	3)	(592	2)	(594	3)	(595	1)	(596	2)
(597	3)								

NAME:13C_1755.8_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176003-11-1

RI:1756

RT: 10.758

NUM PEAKS: 124

(70	30)	(71	81)	(72	51)	(73	1000)	(79	12)
(80	5)	(81	5)	(84	11)	(85	57)	(86	17)
(87	45)	(91	4)	(92	3)	(93	6)	(94	3)
(97	10)	(98	3)	(99	39)	(101	125)	(102	20)
(103	15)	(108	2)	(109	2)	(112	5)	(113	14)
(114	5)	(115	26)	(117	20)	(121	1)	(122	1)
(125	2)	(126	7)	(127	10)	(130	4)	(131	56)
(133	62)	(134	9)	(135	5)	(140	2)	(142	5)

124

(143	18)	(147	245)	(148	47)	(149	22)	(156	2)
(157	4)	(158	16)	(159	21)	(161	7)	(170	3)
(171	10)	(174	12)	(175	50)	(176	9)	(184	6)
(185	7)	(186	5)	(187	7)	(199	3)	(200	9)
(201	4)	(206	19)	(214	5)	(216	5)	(217	16)
(230	5)	(242	4)	(243	15)	(244	6)	(245	4)
(246	4)	(250	1)	(256	11)	(257	69)	(258	282)
(259	63)	(260	23)	(261	4)	(262	3)	(272	2)
(273	9)	(274	45)	(275	9)	(276	4)	(287	9)
(288	4)	(289	3)	(290	3)	(291	1)	(301	2)
(308	1)	(309	1)	(315	1)	(317	3)	(331	6)
(332	6)	(333	8)	(334	5)	(337	2)	(347	3)
(360	5)	(361	21)	(362	79)	(363	23)	(364	10)
(369	1)	(370	1)	(376	7)	(377	9)	(378	3)
(387	1)	(388	1)	(418	1)	(443	2)	(455	1)
(466	1)	(489	2)	(506	1)	(513	1)	(558	1)
(573	1)	(584	1)	(589	1)	(592	1)		

NAME:13C_1761.5_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176004-11-1

RI:1762

RT: 10.791

NUM PEAKS: 88

(70	13)	(73	1000)	(83	4)	(89	102)	(90	22)
(91	5)	(98	5)	(99	44)	(103	42)	(104	95)
(105	41)	(106	5)	(111	1)	(119	73)	(120	7)
(121	2)	(127	5)	(128	8)	(129	28)	(133	68)
(134	35)	(135	8)	(136	1)	(143	8)	(144	10)
(145	214)	(147	114)	(149	14)	(156	2)	(157	4)
(163	11)	(164	2)	(170	1)	(171	3)	(172	12)
(173	26)	(185	4)	(186	5)	(187	4)	(188	13)
(189	60)	(201	4)	(202	6)	(203	19)	(205	20)
(206	8)	(207	36)	(208	5)	(209	2)	(217	7)
(231	7)	(232	2)	(234	24)	(235	500)	(236	57)
(237	19)	(238	1)	(247	3)	(261	1)	(271	1)
(276	2)	(277	5)	(278	1)	(279	2)	(290	2)
(291	2)	(292	2)	(305	1)	(306	1)	(307	1)
(309	1)	(310	6)	(311	1)	(319	1)	(320	3)
(321	18)	(322	4)	(323	1)	(337	4)	(338	3)
(339	1)	(348	1)	(410	2)	(411	7)	(412	2)
(413	1)	(426	1)	(427	2)				

NAME:13C_1796.3_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180001-11-1

RI:1796

RT: 11.063

NUM PEAKS: 145

(70	21)	(71	20)	(72	35)	(73	1000)	(74	95)
(75	235)	(76	17)	(77	12)	(84	8)	(85	17)
(86	11)	(87	38)	(88	133)	(89	79)	(90	19)
(91	6)	(92	2)	(98	9)	(99	101)	(100	16)
(101	23)	(102	17)	(103	68)	(104	117)	(105	88)
(106	11)	(107	3)	(113	4)	(114	4)	(115	19)
(116	13)	(117	15)	(118	44)	(119	71)	(120	8)
(121	2)	(126	1)	(127	7)	(128	12)	(129	11)
(130	10)	(131	32)	(132	71)	(133	85)	(134	27)
(135	7)	(136	1)	(142	2)	(143	5)	(144	12)
(145	22)	(146	15)	(147	142)	(148	32)	(149	27)

125

(150	3)	(151	3)	(156	3)	(157	4)	(158	6)
(159	14)	(160	58)	(161	14)	(162	52)	(163	20)
(164	4)	(166	1)	(172	8)	(173	18)	(174	6)
(177	11)	(178	18)	(179	2)	(183	4)	(187	3)
(188	2)	(189	6)	(191	36)	(192	21)	(199	2)
(200	4)	(202	6)	(203	80)	(204	13)	(205	29)
(206	18)	(207	43)	(208	8)	(209	3)	(217	4)
(218	6)	(219	3)	(220	47)	(221	9)	(222	39)
(223	4)	(224	1)	(230	1)	(231	7)	(232	2)
(233	5)	(234	11)	(235	109)	(236	13)	(237	4)
(240	1)	(246	2)	(247	2)	(248	7)	(249	1)
(263	6)	(264	1)	(275	3)	(276	2)	(277	7)
(278	2)	(279	2)	(281	3)	(282	3)	(290	2)
(291	1)	(296	1)	(305	2)	(306	2)	(308	1)
(309	2)	(310	11)	(311	3)	(312	1)	(320	3)
(321	20)	(322	5)	(323	2)	(324	2)	(325	9)
(326	1)	(336	1)	(337	5)	(338	5)	(351	1)
(352	2)	(381	1)	(411	3)	(412	1)	(427	1)

NAME:13C_3379.6_1313EC07_Lanosta-8,24-dien-3-beta-ol (LTMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:338001-11-1

RI:3380

RT:19.444

NUM PEAKS: 303

(70	50)	(71	29)	(72	235)	(73	810)	(74	1000)
(75	516)	(76	61)	(77	21)	(78	5)	(79	6)
(80	8)	(81	9)	(82	17)	(83	91)	(84	31)
(85	144)	(86	29)	(87	250)	(88	41)	(89	135)
(90	10)	(91	23)	(92	5)	(93	5)	(94	6)
(95	8)	(96	14)	(97	19)	(98	182)	(99	28)
(100	176)	(101	38)	(102	289)	(103	33)	(104	53)
(105	8)	(106	5)	(107	5)	(109	7)	(110	9)
(111	24)	(112	25)	(113	199)	(114	28)	(115	176)
(116	40)	(117	303)	(118	22)	(119	49)	(120	15)
(121	5)	(122	4)	(123	8)	(124	50)	(125	21)
(126	68)	(127	27)	(128	189)	(129	33)	(130	157)
(131	37)	(132	342)	(133	32)	(134	25)	(135	8)
(136	7)	(137	24)	(138	57)	(139	68)	(140	31)
(141	118)	(142	24)	(143	124)	(144	28)	(145	133)
(146	17)	(147	67)	(148	13)	(149	10)	(150	7)
(151	8)	(152	39)	(153	36)	(154	74)	(155	35)
(156	130)	(157	28)	(158	118)	(159	20)	(160	77)
(161	8)	(162	40)	(163	10)	(164	16)	(165	18)
(166	13)	(167	31)	(168	22)	(169	64)	(170	27)
(171	111)	(172	41)	(173	98)	(174	15)	(175	48)
(176	8)	(177	22)	(178	17)	(179	6)	(180	11)
(181	10)	(182	25)	(183	16)	(184	55)	(185	25)
(186	90)	(187	25)	(188	63)	(189	7)	(190	29)
(191	6)	(192	12)	(193	11)	(194	3)	(195	9)
(196	7)	(197	22)	(198	14)	(199	55)	(200	26)
(201	104)	(202	23)	(203	80)	(204	15)	(205	31)
(206	5)	(207	6)	(208	7)	(209	3)	(210	5)
(211	8)	(212	17)	(213	16)	(214	42)	(215	15)
(216	48)	(217	14)	(218	37)	(219	8)	(220	20)
(221	9)	(222	3)	(226	6)	(227	14)	(228	13)
(229	41)	(230	18)	(231	55)	(232	7)	(233	18)
(234	3)	(235	10)	(238	3)	(239	4)	(240	6)
(241	6)	(242	14)	(243	15)	(244	55)	(245	13)
(246	47)	(247	6)	(248	9)	(249	3)	(254	4)

126

(255	5)	(256	5)	(257	15)	(258	20)	(259	79)
(260	12)	(261	24)	(262	6)	(263	5)	(264	3)
(266	4)	(270	4)	(272	10)	(273	8)	(274	35)
(275	5)	(276	21)	(277	5)	(278	3)	(285	5)
(286	5)	(287	10)	(288	6)	(289	17)	(290	8)
(291	12)	(292	10)	(293	6)	(298	3)	(300	4)
(301	6)	(302	12)	(303	7)	(304	11)	(305	5)
(306	6)	(307	5)	(314	3)	(315	3)	(316	5)
(317	8)	(318	6)	(319	10)	(320	3)	(321	6)
(327	3)	(328	3)	(330	3)	(331	4)	(332	9)
(333	4)	(334	14)	(336	3)	(338	3)	(341	3)
(344	3)	(345	3)	(346	6)	(347	11)	(348	4)
(349	7)	(350	5)	(351	4)	(352	4)	(355	3)
(362	7)	(363	3)	(364	5)	(367	3)	(370	3)
(371	4)	(374	3)	(375	4)	(376	7)	(377	7)
(379	4)	(380	4)	(386	4)	(387	4)	(388	3)
(389	3)	(391	3)	(392	3)	(396	3)	(405	3)
(406	3)	(413	3)	(414	3)	(419	7)	(420	19)
(421	53)	(422	149)	(423	29)	(429	3)	(433	3)
(436	3)	(437	5)	(441	3)	(445	4)	(455	3)
(457	3)	(461	3)	(466	3)	(471	3)	(477	3)
(486	3)	(492	4)	(498	3)	(506	3)	(510	8)
(511	17)	(512	37)	(513	20)	(514	6)	(516	3)
(518	3)	(519	5)	(525	4)	(526	10)	(527	16)
(528	36)	(529	16)	(530	4)	(532	3)	(535	3)
(543	4)	(549	3)	(563	3)				

NAME:13C_3079.3_1313EC07

COMMENTS:Kopka J, MPIMP, Dept. Willmützer

CASNO:308001-11-1

RI:3079

RT:18.190

NUM PEAKS: 175

(70	12)	(71	14)	(72	40)	(73	1000)	(74	96)
(75	112)	(76	8)	(77	12)	(83	5)	(84	8)
(85	10)	(86	23)	(87	11)	(88	6)	(89	7)
(90	4)	(91	4)	(96	5)	(97	3)	(98	7)
(99	6)	(100	11)	(101	10)	(102	22)	(103	28)
(104	9)	(105	7)	(107	3)	(111	6)	(112	25)
(113	6)	(114	5)	(115	13)	(116	15)	(117	15)
(118	12)	(119	13)	(121	5)	(123	3)	(124	7)
(125	3)	(126	4)	(129	10)	(130	6)	(131	24)
(132	63)	(133	82)	(134	13)	(135	21)	(136	3)
(137	10)	(138	4)	(139	15)	(140	71)	(141	66)
(142	3)	(143	3)	(144	24)	(145	15)	(146	28)
(147	154)	(148	26)	(149	21)	(150	3)	(151	8)
(152	4)	(153	6)	(154	9)	(155	7)	(158	11)
(159	4)	(160	5)	(161	6)	(162	3)	(165	3)
(167	7)	(168	6)	(169	12)	(170	34)	(172	4)
(173	21)	(174	418)	(175	42)	(176	41)	(177	4)
(179	3)	(180	3)	(181	18)	(182	7)	(183	10)
(184	3)	(189	6)	(190	3)	(191	10)	(192	3)
(193	10)	(194	4)	(195	18)	(196	9)	(197	22)
(198	5)	(199	4)	(205	3)	(206	3)	(207	14)
(208	4)	(209	5)	(210	8)	(211	114)	(212	32)
(213	36)	(214	5)	(218	12)	(219	5)	(220	16)
(222	3)	(223	4)	(224	9)	(225	20)	(226	7)
(227	25)	(228	6)	(229	3)	(233	7)	(234	123)
(235	22)	(236	10)	(240	6)	(241	17)	(242	9)
(243	11)	(247	13)	(248	43)	(249	10)	(250	4)

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(255	7)	(256	7)	(257	15)	(258	3)	(262	9)
(263	65)	(264	16)	(265	6)	(269	5)	(270	7)
(271	7)	(272	19)	(273	3)	(283	4)	(284	3)
(285	8)	(286	3)	(298	8)	(299	76)	(300	24)
(301	12)	(302	3)	(312	4)	(313	8)	(314	25)
(315	214)	(316	66)	(317	30)	(318	6)	(329	3)
(373	3)	(374	8)	(385	3)	(386	19)	(387	11)
(388	6)	(389	3)	(403	5)	(404	15)	(405	3)

NAME:13C_2679.5_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:268001-11-1

RI:2680

RT:16.316

NUM PEAKS: 157

(70	8)	(71	9)	(72	23)	(73	1000)	(74	91)
(75	106)	(76	7)	(77	14)	(83	3)	(84	4)
(85	8)	(86	11)	(87	9)	(88	3)	(89	10)
(90	6)	(91	4)	(98	10)	(99	3)	(100	3)
(101	6)	(102	9)	(103	24)	(104	30)	(105	9)
(106	3)	(107	4)	(113	5)	(114	4)	(115	21)
(116	9)	(117	7)	(118	7)	(119	18)	(121	5)
(129	5)	(130	5)	(131	17)	(132	72)	(133	69)
(134	13)	(135	19)	(136	3)	(137	9)	(139	4)
(140	4)	(141	23)	(144	16)	(145	9)	(146	21)
(147	156)	(148	27)	(149	23)	(150	4)	(151	9)
(158	3)	(159	4)	(160	12)	(161	14)	(162	3)
(163	3)	(165	3)	(174	9)	(175	3)	(176	3)
(177	3)	(178	9)	(179	4)	(181	11)	(182	3)
(183	4)	(188	4)	(189	11)	(190	3)	(191	12)
(192	16)	(193	13)	(194	3)	(195	12)	(196	3)
(197	4)	(202	4)	(203	4)	(205	7)	(206	28)
(207	27)	(208	6)	(209	5)	(210	5)	(211	72)
(212	12)	(213	7)	(217	3)	(218	43)	(219	15)
(220	33)	(225	32)	(226	9)	(227	23)	(228	4)
(233	9)	(234	64)	(235	14)	(236	6)	(242	5)
(243	6)	(248	3)	(255	3)	(256	4)	(260	3)
(262	8)	(263	3)	(269	3)	(276	5)	(277	12)
(278	3)	(283	6)	(284	4)	(285	12)	(286	4)
(298	16)	(299	133)	(300	42)	(301	20)	(302	5)
(313	5)	(314	19)	(315	147)	(316	45)	(317	22)
(318	4)	(328	4)	(329	20)	(330	6)	(331	4)
(343	3)	(344	5)	(351	3)	(358	6)	(359	11)
(360	4)	(372	3)	(373	5)	(374	3)	(375	5)
(386	5)	(387	17)	(388	8)	(389	5)	(429	3)
(445	3)	(446	10)	(447	20)	(448	9)	(449	5)
(450	3)	(518	3)						

NAME:13C_1924.2_1313EC07_Mannitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193002-11-1

RI:1924

RT:12.015

NUM PEAKS: 125

(72	11)	(73	1000)	(74	89)	(75	7)	(87	26)
(89	67)	(90	32)	(91	3)	(100	6)	(101	27)
(102	14)	(103	27)	(104	265)	(105	45)	(106	12)
(114	2)	(115	4)	(116	8)	(117	8)	(118	8)
(119	121)	(120	13)	(121	4)	(128	1)	(129	3)
(130	6)	(131	42)	(132	221)	(133	87)	(134	55)

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(135	9)	(136	1)	(144	1)	(145	4)	(146	17)
(147	472)	(148	66)	(149	39)	(150	3)	(156	2)
(158	2)	(160	6)	(161	150)	(162	162)	(163	41)
(164	12)	(173	4)	(174	9)	(175	2)	(176	6)
(177	12)	(178	8)	(179	1)	(184	1)	(189	1)
(190	9)	(191	50)	(193	2)	(198	2)	(202	2)
(204	5)	(205	3)	(206	8)	(207	234)	(208	46)
(209	21)	(210	1)	(219	10)	(220	95)	(221	22)
(222	10)	(232	2)	(233	44)	(234	10)	(235	41)
(236	11)	(237	17)	(238	3)	(239	1)	(246	4)
(247	2)	(248	7)	(249	6)	(250	4)	(251	3)
(252	1)	(264	3)	(265	2)	(266	2)	(274	8)
(275	3)	(276	1)	(278	9)	(279	14)	(280	6)
(281	1)	(285	1)	(291	1)	(294	14)	(295	6)
(296	2)	(306	2)	(307	2)	(308	2)	(309	5)
(310	5)	(311	4)	(312	1)	(321	1)	(322	16)
(323	206)	(324	72)	(325	33)	(326	6)	(340	2)
(352	2)	(353	1)	(364	1)	(369	1)	(380	1)
(381	4)	(382	2)	(383	1)	(454	1)	(470	1)

NAME:13C_1546.0_1313EC07_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154001-11-1

RI:1546

RT:9.114

NUM PEAKS: 256

(70	14)	(72	42)	(73	1000)	(74	277)	(90	19)
(103	90)	(104	108)	(112	4)	(116	94)	(119	112)
(132	128)	(133	66)	(134	13)	(146	29)	(147	500)
(148	81)	(182	1)	(195	2)	(196	1)	(197	1)
(198	2)	(206	20)	(207	40)	(209	7)	(210	1)
(211	2)	(212	1)	(213	2)	(214	2)	(219	29)
(220	67)	(221	37)	(222	87)	(223	19)	(224	8)
(225	1)	(228	1)	(238	1)	(239	8)	(240	2)
(241	2)	(244	2)	(245	3)	(246	5)	(250	7)
(251	4)	(254	1)	(255	1)	(256	1)	(257	1)
(258	1)	(259	2)	(260	6)	(268	1)	(276	1)
(292	2)	(293	7)	(294	93)	(295	28)	(296	14)
(297	4)	(308	2)	(309	1)	(310	3)	(311	1)
(312	1)	(314	1)	(318	1)	(319	1)	(320	1)
(322	2)	(323	8)	(324	4)	(325	4)	(326	2)
(327	2)	(328	1)	(329	1)	(330	1)	(331	1)
(332	1)	(333	1)	(334	2)	(335	1)	(336	2)
(337	2)	(338	2)	(339	2)	(340	2)	(341	2)
(342	2)	(343	2)	(344	2)	(345	2)	(346	2)
(347	2)	(348	2)	(349	2)	(350	1)	(351	1)
(352	2)	(353	3)	(354	1)	(355	2)	(356	2)
(357	1)	(358	1)	(359	1)	(360	1)	(361	1)
(362	1)	(363	1)	(364	1)	(365	1)	(366	1)
(367	1)	(368	1)	(369	1)	(370	1)	(375	1)
(380	1)	(381	1)	(382	3)	(383	2)	(384	1)
(385	1)	(387	1)	(398	1)	(406	1)	(407	1)
(412	2)	(413	5)	(414	3)	(415	2)	(416	1)
(418	1)	(419	1)	(420	1)	(421	1)	(422	1)
(423	1)	(424	1)	(425	1)	(426	1)	(427	1)
(428	1)	(429	1)	(430	1)	(431	1)	(432	1)
(433	1)	(434	1)	(435	1)	(436	1)	(438	2)
(439	1)	(440	2)	(441	1)	(442	1)	(443	1)
(444	1)	(445	1)	(446	1)	(448	1)	(449	1)
(450	1)	(451	1)	(452	1)	(453	2)	(454	1)

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(455	2)	(456	1)	(457	1)	(458	1)	(460	1)
(461	1)	(463	1)	(464	1)	(466	1)	(467	1)
(468	1)	(469	1)	(470	1)	(471	1)	(472	1)
(474	1)	(475	1)	(477	1)	(478	1)	(480	1)
(481	1)	(485	1)	(486	1)	(490	1)	(491	1)
(492	1)	(495	1)	(501	1)	(504	1)	(505	1)
(509	1)	(512	1)	(515	1)	(516	1)	(519	2)
(520	1)	(522	1)	(523	1)	(524	2)	(525	2)
(526	1)	(528	1)	(529	1)	(530	1)	(531	1)
(532	1)	(533	1)	(534	1)	(535	1)	(536	1)
(537	1)	(538	1)	(539	1)	(540	1)	(541	1)
(542	1)	(543	1)	(544	1)	(545	1)	(546	1)
(547	1)	(548	1)	(549	1)	(550	1)	(551	1)
(552	1)	(554	1)	(555	1)	(556	1)	(557	1)
(558	1)	(559	1)	(560	1)	(561	1)	(563	1)
(564	1)	(566	1)	(567	1)	(568	1)	(570	1)
(571	1)	(572	1)	(573	1)	(574	1)	(584	1)
(586	1)								

NAME:13C_1281.6_1313EC07_Ethanolamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RT:1282

CASNO:128002-11-1

RI:1282

RT:6.144

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 147

(79	93)	(87	108)	(94	16)	(100	30)	(101	24)
(112	6)	(113	33)	(124	14)	(126	7)	(138	42)
(144	15)	(157	11)	(160	5)	(161	5)	(172	6)
(174	36)	(175	1000)	(176	177)	(180	30)	(183	4)
(190	1)	(198	5)	(202	3)	(203	11)	(204	29)
(212	6)	(217	9)	(222	2)	(231	9)	(233	4)
(242	15)	(244	26)	(245	13)	(252	15)	(260	6)
(262	26)	(263	15)	(264	19)	(276	8)	(277	4)
(279	20)	(281	42)	(282	13)	(284	28)	(287	5)
(291	12)	(296	10)	(298	27)	(306	24)	(307	6)
(309	3)	(313	30)	(322	15)	(324	2)	(328	22)
(333	6)	(335	40)	(336	41)	(343	16)	(344	5)
(346	1)	(347	13)	(349	17)	(354	27)	(355	18)
(360	19)	(361	34)	(362	15)	(363	10)	(364	9)
(368	1)	(369	26)	(372	13)	(374	20)	(376	41)
(388	14)	(393	16)	(398	11)	(399	15)	(401	3)
(402	7)	(405	16)	(406	6)	(408	9)	(409	17)
(410	61)	(414	12)	(415	2)	(416	40)	(421	6)
(422	12)	(426	9)	(427	6)	(434	11)	(438	27)
(441	11)	(444	7)	(448	9)	(452	1)	(453	5)
(455	10)	(459	33)	(460	21)	(463	10)	(467	30)
(470	2)	(471	40)	(472	3)	(473	7)	(480	32)
(484	19)	(485	6)	(489	32)	(490	22)	(491	23)
(493	15)	(494	42)	(498	29)	(505	3)	(513	21)
(514	32)	(517	28)	(520	27)	(522	10)	(525	1)
(529	31)	(534	6)	(541	22)	(542	8)	(554	5)
(557	3)	(558	13)	(559	5)	(561	11)	(572	3)
(573	9)	(577	29)	(579	12)	(582	4)	(583	21)
(587	4)	(588	5)	(592	14)	(593	6)	(595	12)
(598	3)	(599	12)						

NAME:13C_1283.2_1313EC11_Urea (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:127002-11-1

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RI:1283

RT:6.186

NUM PEAKS: 410

(70	54)	(71	41)	(72	86)	(73	263)	(74	200)
(75	57)	(76	9)	(77	9)	(78	36)	(79	62)
(80	10)	(82	5)	(83	4)	(84	5)	(85	14)
(86	27)	(87	54)	(90	9)	(92	6)	(93	9)
(94	8)	(95	6)	(97	7)	(98	4)	(99	26)
(100	103)	(101	95)	(102	33)	(103	25)	(105	6)
(107	7)	(108	7)	(109	5)	(111	5)	(112	9)
(113	12)	(114	12)	(115	29)	(116	41)	(117	17)
(121	5)	(122	6)	(123	12)	(125	14)	(126	13)
(127	5)	(128	9)	(129	9)	(130	71)	(131	76)
(132	88)	(133	25)	(137	7)	(138	5)	(139	5)
(140	7)	(141	5)	(142	5)	(143	8)	(144	8)
(146	62)	(147	1000)	(148	210)	(149	90)	(150	14)
(151	5)	(152	7)	(153	7)	(154	6)	(155	6)
(156	7)	(157	8)	(158	11)	(159	7)	(160	10)
(163	9)	(164	8)	(167	6)	(168	7)	(169	4)
(170	6)	(171	38)	(172	101)	(173	33)	(174	45)
(177	8)	(178	8)	(179	5)	(180	5)	(182	5)
(183	3)	(184	5)	(185	7)	(186	5)	(187	8)
(188	6)	(189	98)	(190	259)	(191	51)	(192	27)
(193	7)	(194	6)	(195	5)	(196	6)	(197	4)
(198	7)	(200	4)	(203	3)	(204	12)	(205	17)
(206	10)	(207	8)	(208	5)	(209	4)	(212	5)
(213	6)	(214	5)	(215	5)	(216	5)	(217	6)
(218	5)	(220	5)	(222	10)	(223	5)	(224	5)
(225	5)	(226	8)	(227	4)	(229	6)	(230	8)
(231	7)	(232	5)	(233	5)	(234	5)	(235	6)
(236	7)	(238	4)	(239	8)	(240	7)	(242	3)
(243	5)	(244	6)	(245	5)	(247	3)	(248	5)
(249	4)	(250	2)	(251	5)	(252	6)	(254	4)
(256	3)	(257	6)	(258	5)	(259	5)	(260	4)
(261	3)	(263	5)	(264	5)	(265	6)	(266	4)
(267	6)	(268	7)	(269	8)	(270	7)	(271	10)
(272	6)	(273	6)	(275	16)	(276	8)	(277	8)
(278	8)	(279	8)	(280	7)	(281	6)	(283	5)
(284	5)	(287	8)	(288	8)	(289	11)	(290	7)
(292	4)	(293	10)	(294	6)	(295	5)	(296	4)
(297	6)	(298	4)	(300	4)	(301	3)	(302	4)
(303	6)	(304	3)	(306	3)	(307	2)	(308	4)
(309	5)	(310	4)	(312	6)	(314	6)	(315	5)
(316	7)	(317	7)	(318	5)	(319	6)	(320	5)
(322	3)	(323	6)	(326	7)	(327	5)	(328	8)
(329	6)	(330	6)	(331	3)	(332	6)	(333	7)
(334	5)	(335	4)	(336	5)	(337	5)	(339	5)
(340	5)	(341	2)	(342	5)	(343	7)	(344	4)
(345	4)	(346	5)	(347	9)	(348	6)	(349	4)
(351	6)	(352	6)	(353	5)	(354	7)	(355	8)
(357	6)	(358	7)	(359	8)	(360	11)	(361	9)
(362	8)	(363	5)	(364	13)	(365	6)	(366	6)
(367	8)	(368	5)	(369	7)	(371	9)	(373	5)
(374	3)	(375	7)	(376	7)	(377	6)	(378	8)
(379	13)	(380	5)	(381	5)	(383	9)	(389	11)
(391	5)	(392	5)	(393	6)	(394	4)	(395	7)
(397	5)	(398	5)	(400	6)	(401	5)	(402	6)
(403	5)	(404	5)	(405	6)	(406	4)	(407	3)
(408	5)	(409	4)	(410	6)	(411	9)	(412	5)
(415	6)	(416	5)	(417	6)	(419	6)	(420	4)

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(421	6)	(422	4)	(423	3)	(424	3)	(426	4)
(427	6)	(430	4)	(431	3)	(432	5)	(433	6)
(434	5)	(435	6)	(437	5)	(438	3)	(440	6)
(441	5)	(442	4)	(444	4)	(445	5)	(446	5)
(447	5)	(448	7)	(449	4)	(450	6)	(451	5)
(454	5)	(455	4)	(457	4)	(458	6)	(459	5)
(460	6)	(461	5)	(462	6)	(463	9)	(464	5)
(466	3)	(467	5)	(468	3)	(469	3)	(470	8)
(471	8)	(472	8)	(473	7)	(475	2)	(476	6)
(477	7)	(479	6)	(480	5)	(482	7)	(484	7)
(486	5)	(487	17)	(489	7)	(490	5)	(491	6)
(492	5)	(493	5)	(495	3)	(498	8)	(499	7)
(500	6)	(501	4)	(502	5)	(503	6)	(504	5)
(505	6)	(506	6)	(507	7)	(508	4)	(510	5)
(511	3)	(512	2)	(513	6)	(514	5)	(515	6)
(516	5)	(517	5)	(518	6)	(519	8)	(522	6)
(523	5)	(524	5)	(525	6)	(528	3)	(529	5)
(530	5)	(531	4)	(532	6)	(533	6)	(534	7)
(536	3)	(537	6)	(539	4)	(540	7)	(541	7)
(542	4)	(544	6)	(545	6)	(546	3)	(547	5)
(548	7)	(551	3)	(552	5)	(553	3)	(554	4)
(555	7)	(556	4)	(561	5)	(562	3)	(563	6)
(564	4)	(566	6)	(567	5)	(568	4)	(569	4)
(572	5)	(574	2)	(575	5)	(577	3)	(579	3)
(582	2)	(588	3)	(589	2)	(590	3)	(591	3)

NAME:13C_2223.0_1313EC16_Tryptophan (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223001-11-1

RI:2223

RT:13.883

NUM PEAKS: 161

(72	59)	(73	320)	(74	110)	(75	153)	(76	19)
(80	12)	(87	41)	(88	38)	(89	48)	(95	15)
(101	36)	(102	56)	(110	28)	(116	8)	(120	9)
(124	8)	(130	8)	(136	10)	(137	23)	(138	38)
(139	22)	(141	18)	(143	10)	(151	7)	(153	12)
(157	7)	(162	12)	(167	7)	(170	4)	(173	7)
(174	5)	(175	11)	(177	8)	(179	15)	(195	6)
(196	7)	(197	8)	(200	4)	(203	14)	(204	11)
(209	27)	(210	108)	(211	1000)	(212	79)	(213	28)
(216	7)	(217	7)	(219	6)	(229	5)	(231	4)
(232	5)	(237	11)	(240	8)	(247	4)	(249	5)
(251	6)	(258	7)	(259	4)	(263	5)	(270	5)
(274	5)	(276	3)	(280	6)	(281	5)	(290	4)
(291	6)	(292	5)	(294	3)	(295	4)	(307	3)
(313	5)	(314	7)	(316	5)	(317	5)	(329	2)
(330	4)	(334	4)	(335	4)	(351	5)	(352	2)
(353	4)	(355	7)	(373	4)	(378	3)	(379	4)
(384	3)	(386	4)	(388	3)	(391	3)	(396	4)
(397	4)	(405	3)	(407	6)	(408	6)	(410	4)
(413	5)	(417	6)	(418	5)	(422	9)	(424	4)
(425	2)	(426	6)	(427	2)	(431	3)	(433	4)
(438	3)	(441	4)	(442	4)	(445	3)	(446	5)
(447	5)	(448	3)	(455	4)	(462	4)	(465	4)
(467	1)	(471	6)	(475	4)	(477	5)	(479	2)
(481	3)	(482	5)	(486	4)	(488	5)	(489	5)
(493	3)	(496	7)	(497	4)	(498	3)	(499	4)
(500	3)	(502	3)	(509	3)	(513	3)	(516	4)
(517	2)	(518	2)	(520	4)	(523	4)	(527	2)

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(532	4)	(536	4)	(537	2)	(538	4)	(541	4)
(542	3)	(543	6)	(546	3)	(547	3)	(550	2)
(552	4)	(555	3)	(558	2)	(564	3)	(566	3)
(567	4)	(571	2)	(573	2)	(574	2)	(591	2)
(595	2)								

NAME:13C_2767.9_1313EC16

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:277004-11-1

RI:2767

RT:16.765

NUM PEAKS: 93

(70	41)	(72	34)	(73	1000)	(74	107)	(76	39)
(78	24)	(82	14)	(83	31)	(84	35)	(91	22)
(92	19)	(93	18)	(97	17)	(98	22)	(99	25)
(100	21)	(102	40)	(103	55)	(105	32)	(106	48)
(107	56)	(111	34)	(112	80)	(113	31)	(117	32)
(118	68)	(124	32)	(126	12)	(127	18)	(129	47)
(131	35)	(138	16)	(139	31)	(140	162)	(141	348)
(142	16)	(145	24)	(146	55)	(151	18)	(152	13)
(153	15)	(154	42)	(155	21)	(167	11)	(168	21)
(169	148)	(170	718)	(171	19)	(173	18)	(174	266)
(176	24)	(178	130)	(179	769)	(180	79)	(181	67)
(183	20)	(193	399)	(194	30)	(195	33)	(196	13)
(197	33)	(198	18)	(206	179)	(207	48)	(211	32)
(212	26)	(213	52)	(214	15)	(215	10)	(216	12)
(223	15)	(224	17)	(241	23)	(243	12)	(249	26)
(254	10)	(270	18)	(271	20)	(272	22)	(273	35)
(274	12)	(282	12)	(283	12)	(347	10)	(348	12)
(385	11)	(404	17)	(405	10)	(429	8)	(436	11)
(437	18)	(494	10)	(523	15)				

NAME:13C_1915.4_2119DC05_Lysine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192003-11-1

RI:1915

RT:28.691

NUM PEAKS: 222

(40	3)	(41	58)	(42	5)	(43	19)	(44	18)
(45	84)	(46	5)	(47	6)	(50	2)	(51	8)
(52	5)	(53	14)	(54	2)	(55	59)	(56	10)
(57	104)	(58	19)	(59	126)	(60	15)	(61	8)
(62	1)	(63	4)	(64	3)	(65	13)	(66	5)
(67	20)	(68	2)	(69	8)	(70	3)	(72	25)
(73	1000)	(74	116)	(75	82)	(76	7)	(77	23)
(78	6)	(79	20)	(80	3)	(81	9)	(82	3)
(83	6)	(86	12)	(87	139)	(88	21)	(89	85)
(90	5)	(91	34)	(92	4)	(93	8)	(94	2)
(95	10)	(96	4)	(97	5)	(98	2)	(100	20)
(101	91)	(102	73)	(103	58)	(105	15)	(106	3)
(107	11)	(108	2)	(109	18)	(110	4)	(111	6)
(112	1)	(114	7)	(115	55)	(116	29)	(117	127)
(118	23)	(120	3)	(121	10)	(122	2)	(123	8)
(124	5)	(126	1)	(127	3)	(128	16)	(129	37)
(130	64)	(131	270)	(132	51)	(133	59)	(134	8)
(135	19)	(136	5)	(137	8)	(138	2)	(139	2)
(140	1)	(141	4)	(142	4)	(143	11)	(144	11)
(145	58)	(146	65)	(147	126)	(148	29)	(149	21)
(150	7)	(151	5)	(152	3)	(153	7)	(154	8)
(155	2)	(156	14)	(157	8)	(158	7)	(159	68)

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(160	59)	(161	691)	(162	55)	(163	36)	(164	5)
(165	5)	(166	1)	(167	1)	(170	1)	(171	3)
(172	11)	(173	24)	(175	666)	(176	117)	(177	85)
(178	13)	(179	6)	(180	1)	(185	2)	(186	3)
(187	8)	(188	6)	(189	58)	(190	23)	(191	16)
(192	26)	(193	5)	(194	3)	(199	1)	(200	2)
(201	7)	(202	5)	(203	66)	(204	22)	(205	98)
(206	21)	(213	1)	(215	2)	(217	53)	(218	39)
(219	18)	(220	66)	(221	17)	(222	8)	(223	1)
(228	1)	(229	1)	(230	3)	(231	3)	(232	21)
(233	66)	(234	124)	(235	50)	(236	15)	(237	2)
(238	1)	(243	1)	(244	1)	(245	3)	(246	5)
(247	4)	(249	4)	(250	1)	(251	1)	(257	1)
(260	1)	(261	16)	(262	5)	(263	2)	(264	4)
(265	2)	(271	1)	(276	3)	(277	3)	(278	8)
(279	7)	(280	2)	(291	1)	(292	1)	(299	9)
(300	2)	(301	1)	(305	1)	(306	1)	(307	2)
(308	2)	(309	1)	(317	3)	(318	1)	(319	1)
(320	1)	(321	6)	(322	174)	(323	39)	(324	21)
(325	4)	(326	1)	(333	1)	(334	1)	(335	17)
(336	7)	(337	3)	(396	3)	(397	1)	(425	4)
(426	1)	(427	1)	(439	1)	(440	19)	(441	7)
(442	4)	(443	1)						

NAME:13C_1920.1_2119DC05_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192007-11-1

RI:1920

RT:28.753

NUM PEAKS: 81

(43	35)	(44	17)	(45	80)	(47	12)	(58	64)
(71	61)	(72	24)	(73	1000)	(74	88)	(75	149)
(76	8)	(84	12)	(85	35)	(86	15)	(113	7)
(118	24)	(131	28)	(132	22)	(133	36)	(140	3)
(147	445)	(148	62)	(149	62)	(160	17)	(169	6)
(174	17)	(203	35)	(204	5)	(206	14)	(221	34)
(223	5)	(229	3)	(231	6)	(247	3)	(248	153)
(249	33)	(250	18)	(259	2)	(263	3)	(264	12)
(277	20)	(278	7)	(279	5)	(290	2)	(291	4)
(292	8)	(293	303)	(294	56)	(295	29)	(296	4)
(297	2)	(305	3)	(306	12)	(307	13)	(308	11)
(309	4)	(311	4)	(319	32)	(320	12)	(321	8)
(324	6)	(338	12)	(339	3)	(352	12)	(353	6)
(354	3)	(366	4)	(367	68)	(368	20)	(369	7)
(370	3)	(378	2)	(383	32)	(384	8)	(385	4)
(396	22)	(397	5)	(468	3)	(486	27)	(487	8)
(488	5)								

NAME:13C_1858.1_2119DC05_Lysine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858

CASNO:186002-11-1

RI:1858

RT:27.441

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 119

(44	26)	(45	125)	(46	12)	(47	13)	(48	1)
(50	1)	(51	1)	(52	2)	(58	15)	(59	185)
(60	20)	(61	11)	(62	1)	(70	3)	(72	19)
(73	789)	(74	139)	(76	11)	(78	1)	(85	4)
(86	13)	(87	199)	(88	34)	(89	233)	(90	7)

134

(91	2)	(92	1)	(100	27)	(101	85)	(102	28)
(103	33)	(104	19)	(106	1)	(110	1)	(113	4)
(114	6)	(115	21)	(116	16)	(118	15)	(119	8)
(120	2)	(128	2)	(130	47)	(131	76)	(133	25)
(134	5)	(135	2)	(142	1)	(144	4)	(146	49)
(147	72)	(148	26)	(149	9)	(150	2)	(156	3)
(157	1)	(158	2)	(159	13)	(160	18)	(161	210)
(162	25)	(163	11)	(164	2)	(172	6)	(173	28)
(174	66)	(175	1000)	(176	170)	(177	80)	(178	9)
(179	2)	(188	3)	(189	10)	(190	12)	(192	9)
(193	2)	(200	3)	(202	1)	(203	14)	(204	5)
(205	13)	(206	176)	(207	20)	(208	8)	(217	1)
(218	2)	(219	2)	(220	9)	(230	1)	(232	1)
(233	2)	(234	4)	(235	30)	(236	8)	(237	3)
(238	1)	(245	6)	(246	2)	(247	2)	(248	3)
(249	2)	(250	1)	(261	2)	(262	1)	(263	6)
(264	47)	(265	8)	(266	4)	(278	1)	(294	1)
(295	6)	(296	1)	(297	1)	(336	1)	(353	2)
(367	1)	(368	20)	(369	5)	(370	2)		

NAME:13C_1490.2_2119DC05_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149003-11-1

RI:1490

RT:20.226

NUM PEAKS: 155

(42	41)	(43	38)	(44	220)	(45	159)	(46	109)
(47	38)	(51	16)	(52	19)	(56	10)	(57	23)
(59	236)	(60	49)	(61	112)	(62	15)	(64	3)
(65	3)	(66	11)	(69	8)	(70	14)	(71	8)
(72	76)	(73	1000)	(74	208)	(75	701)	(76	80)
(77	52)	(79	27)	(80	4)	(85	8)	(86	20)
(87	35)	(88	54)	(89	68)	(90	253)	(91	31)
(92	26)	(94	9)	(99	4)	(100	14)	(101	70)
(102	28)	(104	27)	(107	5)	(113	5)	(115	13)
(116	12)	(117	25)	(118	91)	(119	64)	(122	6)
(126	7)	(129	12)	(130	16)	(132	12)	(134	36)
(135	20)	(145	14)	(146	75)	(147	952)	(148	301)
(149	96)	(150	15)	(155	3)	(158	7)	(160	4)
(161	19)	(162	116)	(163	119)	(164	154)	(165	40)
(166	17)	(174	3)	(179	14)	(180	7)	(181	5)
(183	2)	(192	191)	(193	50)	(194	21)	(195	3)
(196	5)	(200	3)	(202	3)	(204	5)	(208	40)
(209	146)	(210	26)	(211	17)	(216	2)	(220	19)
(222	5)	(224	6)	(235	21)	(237	41)	(239	3)
(241	2)	(242	3)	(252	14)	(253	67)	(254	13)
(255	8)	(256	3)	(258	2)	(260	3)	(264	3)
(271	3)	(279	3)	(280	10)	(281	135)	(282	26)
(283	16)	(284	2)	(285	2)	(287	3)	(295	3)
(297	7)	(298	30)	(299	4)	(300	9)	(303	2)
(322	4)	(327	26)	(328	7)	(329	4)	(342	2)
(345	3)	(346	2)	(349	3)	(350	2)	(354	2)
(358	3)	(407	4)	(412	3)	(413	3)	(433	2)
(445	3)	(447	5)	(449	4)	(454	3)	(459	2)
(463	2)	(474	2)	(478	3)	(491	2)	(495	2)
(503	3)	(512	2)	(533	2)	(545	2)	(553	3)
(556	2)	(562	2)	(568	3)	(570	3)	(597	3)

NAME:13C_2816.0_2119DC05_

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:282003-11-1

RI:2816

RT:41.157

NUM PEAKS: 36

(46	17)	(73	1000)	(74	77)	(75	76)	(104	215)
(132	227)	(133	65)	(147	285)	(148	36)	(160	54)
(161	50)	(174	153)	(178	14)	(186	13)	(188	11)
(192	358)	(193	75)	(194	44)	(206	128)	(208	24)
(218	14)	(220	305)	(221	69)	(222	23)	(233	22)
(236	22)	(248	74)	(263	13)	(277	83)	(308	25)
(323	33)	(336	46)	(367	386)	(368	92)	(369	49)
(370	12)								

NAME:12C_1731.5_1313EC36_Ribitol (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173001-10-1

RI:1731

RT:10.548

NUM PEAKS: 84

(70	4)	(71	5)	(72	21)	(73	1000)	(74	87)
(75	73)	(76	3)	(77	3)	(81	8)	(83	5)
(85	4)	(87	8)	(88	6)	(89	28)	(90	3)
(99	5)	(101	28)	(102	5)	(103	225)	(104	22)
(105	10)	(111	3)	(113	6)	(115	6)	(116	10)
(117	95)	(118	9)	(119	9)	(129	129)	(130	16)
(131	33)	(132	5)	(133	70)	(134	10)	(135	6)
(142	3)	(143	10)	(145	4)	(147	309)	(148	49)
(149	31)	(150	3)	(155	6)	(157	24)	(158	3)
(159	3)	(161	3)	(163	5)	(170	3)	(171	3)
(175	6)	(177	3)	(189	55)	(190	12)	(191	24)
(192	4)	(203	14)	(204	48)	(205	106)	(206	22)
(207	12)	(217	242)	(218	65)	(219	25)	(220	4)
(221	9)	(229	7)	(231	3)	(243	15)	(244	4)
(277	10)	(278	4)	(291	4)	(306	4)	(307	30)
(308	9)	(309	4)	(317	5)	(318	5)	(319	50)
(320	16)	(321	7)	(332	10)	(333	4)		

NAME:12C_1316.0_1313EC36_Isoleucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:132002-10-1

RI:1316

RT:6.560

NUM PEAKS: 44

(70	19)	(71	7)	(72	26)	(73	895)	(82	4)
(84	12)	(85	11)	(86	48)	(89	4)	(90	8)
(96	6)	(97	4)	(98	12)	(99	7)	(100	126)
(102	39)	(103	21)	(105	3)	(112	5)	(113	4)
(126	3)	(128	27)	(129	20)	(133	34)	(134	8)
(145	3)	(147	137)	(149	16)	(156	7)	(158	1000)
(159	149)	(160	48)	(161	5)	(163	5)	(170	15)
(171	3)	(174	3)	(203	9)	(217	3)	(218	142)
(232	38)	(233	12)	(260	7)	(261	2)		

NAME:12C_1436.0_1313EC36_[619; 2-(3',4'-Bishydroxyphenyl)-2-oxoethylamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:143003-10-1

RI:1436

RT:7.989

NUM PEAKS: 26

136

(73 1000) (74 109) (82 77) (85 30) (86 334)
 (87 39) (89 58) (99 28) (100 186) (102 163)
 (113 38) (114 26) (117 29) (126 26) (128 32)
 (130 75) (154 393) (155 90) (156 130) (158 17)
 (172 55) (174 538) (175 96) (176 35) (186 32)
 (227 34)

NAME:12C_1459.3_1313EC36_Homoserine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146001-10-1

RI:1459

RT:8.266

NUM PEAKS: 72

(70 8) (71 13) (72 26) (73 1000) (74 95)
 (75 119) (76 11) (77 5) (82 6) (83 3)
 (84 15) (85 5) (86 10) (87 9) (88 4)
 (98 11) (100 107) (101 22) (102 45) (103 235)
 (104 23) (105 12) (112 8) (113 4) (114 14)
 (115 8) (116 7) (117 15) (119 7) (127 4)
 (128 397) (129 58) (130 63) (131 43) (132 25)
 (133 62) (134 10) (135 5) (137 3) (143 4)
 (144 6) (145 3) (146 19) (156 7) (158 9)
 (160 4) (163 4) (172 6) (174 10) (175 4)
 (176 4) (178 3) (186 4) (188 8) (189 4)
 (191 3) (202 32) (203 8) (204 6) (214 4)
 (216 11) (217 6) (218 503) (219 112) (220 42)
 (221 8) (230 17) (231 4) (232 8) (292 17)
 (293 6) (320 6)

NAME:12C_1495.6_1313EC36_[815; Ethyl-3(2H)-thiophenone]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150003-10-1

RI:1496

RT:8.698

NUM PEAKS: 56

(72 18) (73 546) (74 61) (75 165) (76 13)
 (77 10) (82 5) (84 10) (86 11) (87 6)
 (88 3) (96 3) (98 18) (100 67) (101 12)
 (102 9) (103 16) (104 3) (105 3) (112 9)
 (114 16) (115 12) (116 8) (117 41) (118 5)
 (119 5) (126 5) (128 1000) (129 133) (130 82)
 (131 18) (132 10) (133 23) (134 4) (144 5)
 (146 3) (148 11) (149 13) (156 7) (158 13)
 (172 4) (173 3) (174 5) (188 94) (189 13)
 (190 4) (200 3) (202 60) (203 12) (204 5)
 (216 3) (218 10) (219 3) (230 12) (290 4)
 (305 3)

NAME:12C_1514.1_1313EC36_[729; N,N-Dimethyllysine methyl ester]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151003-10-1

RI:1514

RT:8.860

NUM PEAKS: 29

(72 40) (73 1000) (74 101) (75 258) (82 16)
 (84 893) (87 12) (89 205) (98 119) (100 81)
 (105 28) (114 32) (116 18) (128 67) (131 30)
 (133 46) (140 41) (147 188) (148 29) (156 104)
 (157 14) (158 35) (172 23) (188 844) (189 112)
 (190 28) (200 16) (230 29) (274 20)

137

NAME:12C_1538.2_1313EC36_[596; N-Acetylglutamic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154002-10-1

RI:1538

RT:9.048

NUM PEAKS: 61

(72	46)	(73	454)	(74	75)	(75	623)	(76	52)
(77	33)	(83	17)	(84	1000)	(86	12)	(87	18)
(88	13)	(89	9)	(90	3)	(91	6)	(101	19)
(102	10)	(103	18)	(104	3)	(112	10)	(114	7)
(115	7)	(116	31)	(118	4)	(129	25)	(130	34)
(131	24)	(132	5)	(133	22)	(134	3)	(140	40)
(141	6)	(142	9)	(143	3)	(144	12)	(145	14)
(146	19)	(147	62)	(148	10)	(149	13)	(156	57)
(157	15)	(158	202)	(159	30)	(160	13)	(173	21)
(174	400)	(175	52)	(176	16)	(186	68)	(187	8)
(201	17)	(202	3)	(230	35)	(231	8)	(232	3)
(248	14)	(249	3)	(258	4)	(276	33)	(277	7)
(278	3)								

NAME:12C_1623.5_1313EC36_[882; Ornithine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:162001-10-1

RI:1624

RT:9.710

NUM PEAKS: 109

(70	553)	(71	37)	(72	35)	(73	1000)	(74	231)
(75	128)	(76	13)	(77	5)	(80	4)	(82	5)
(83	4)	(84	13)	(85	10)	(86	21)	(87	12)
(88	15)	(89	26)	(90	7)	(96	7)	(97	14)
(98	20)	(99	9)	(100	96)	(101	19)	(102	115)
(103	26)	(104	11)	(105	3)	(108	3)	(110	5)
(112	6)	(113	6)	(114	24)	(115	75)	(116	19)
(117	41)	(118	7)	(119	5)	(126	9)	(127	4)
(128	65)	(129	30)	(130	32)	(131	25)	(132	29)
(133	34)	(134	7)	(135	3)	(140	9)	(141	10)
(142	661)	(143	104)	(144	92)	(145	12)	(146	22)
(147	108)	(148	34)	(149	14)	(150	3)	(152	3)
(153	16)	(154	13)	(155	4)	(157	7)	(158	7)
(159	5)	(160	4)	(162	60)	(163	11)	(164	5)
(168	3)	(169	14)	(170	8)	(171	5)	(172	9)
(173	3)	(174	7)	(186	4)	(187	4)	(188	9)
(189	5)	(190	3)	(191	4)	(200	7)	(203	3)
(204	43)	(205	9)	(206	4)	(214	4)	(215	5)
(216	33)	(217	16)	(218	22)	(219	9)	(220	3)
(227	4)	(231	7)	(232	8)	(233	3)	(241	4)
(243	31)	(244	27)	(245	8)	(258	7)	(259	12)
(260	3)	(348	27)	(349	9)	(350	4)		

NAME:12C_1640.8_1313EC36_Phenylalanine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:164001-10-1

RI:1641

RT:9.844

NUM PEAKS: 63

(71	5)	(72	21)	(73	1000)	(74	94)	(75	110)
(76	8)	(77	15)	(78	5)	(86	18)	(87	6)
(89	12)	(90	6)	(91	174)	(92	26)	(93	5)
(100	189)	(101	26)	(103	21)	(104	5)	(105	7)

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(115	8)	(116	3)	(117	15)	(118	10)	(119	10)
(120	12)	(121	9)	(130	41)	(131	26)	(132	31)
(133	34)	(134	7)	(135	9)	(145	5)	(146	12)
(147	159)	(148	27)	(149	15)	(159	5)	(160	18)
(161	5)	(162	7)	(163	10)	(174	5)	(176	10)
(177	12)	(178	3)	(190	3)	(191	7)	(192	282)
(193	53)	(194	13)	(203	7)	(204	11)	(205	3)
(217	4)	(218	397)	(219	77)	(220	33)	(266	24)
(267	13)	(268	4)	(294	6)				

NAME:12C_1673.2_1313EC36_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167003-10-1

RI:1673

RT:10.095

NUM PEAKS: 66

(70	28)	(73	1000)	(74	100)	(82	142)	(84	9)
(98	500)	(99	37)	(101	8)	(110	18)	(114	17)
(116	11)	(130	10)	(140	5)	(154	5)	(156	50)
(157	11)	(170	36)	(176	4)	(184	14)	(186	4)
(198	5)	(199	4)	(200	13)	(216	9)	(221	5)
(230	4)	(231	10)	(232	9)	(244	14)	(249	4)
(252	4)	(267	5)	(279	4)	(287	21)	(288	458)
(289	117)	(290	45)	(291	8)	(293	5)	(318	6)
(319	6)	(322	4)	(324	4)	(336	7)	(337	4)
(344	4)	(346	10)	(347	6)	(391	5)	(398	4)
(408	5)	(409	4)	(410	5)	(423	5)	(431	5)
(439	4)	(447	4)	(478	4)	(481	6)	(490	5)
(515	5)	(532	4)	(548	4)	(558	4)	(567	3)
(570	3)								

NAME:12C_1708.2_1313EC36_[499; 2-Ethyl-3-hydroxy-3-methylvaleric acid
(2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:171003-10-1

RI:1708

RT:10.367

NUM PEAKS: 91

(70	22)	(71	9)	(72	25)	(73	1000)	(74	81)
(75	114)	(79	9)	(81	14)	(86	12)	(87	8)
(89	87)	(100	46)	(105	5)	(112	7)	(114	16)
(116	19)	(117	15)	(127	24)	(128	52)	(129	21)
(132	16)	(133	28)	(134	6)	(135	3)	(142	28)
(143	8)	(144	24)	(145	32)	(146	9)	(147	91)
(148	13)	(149	6)	(155	61)	(158	11)	(159	5)
(161	10)	(171	62)	(172	19)	(174	22)	(175	4)
(176	5)	(182	5)	(183	5)	(185	9)	(187	6)
(188	11)	(202	8)	(211	8)	(218	16)	(219	17)
(228	6)	(229	9)	(232	13)	(242	3)	(243	5)
(244	24)	(245	12)	(246	4)	(272	31)	(275	102)
(276	28)	(277	12)	(287	5)	(288	6)	(296	9)
(297	6)	(298	7)	(337	4)	(338	4)	(348	6)
(350	6)	(358	3)	(399	4)	(411	4)	(415	5)
(421	4)	(422	4)	(431	4)	(458	6)	(459	4)
(462	4)	(470	3)	(479	4)	(483	5)	(513	5)
(515	5)	(543	5)	(548	7)	(557	5)	(558	4)
(588	4)								

NAME:12C_1720.9_1313EC36_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:172005-10-1

RI:1721

RT:10.465

NUM PEAKS: 56

(70	46)	(72	90)	(73	789)	(74	188)	(75	1000)
(76	84)	(77	54)	(81	16)	(83	199)	(86	17)
(87	41)	(90	180)	(94	9)	(112	17)	(113	31)
(115	83)	(116	152)	(119	8)	(126	11)	(131	167)
(132	24)	(139	70)	(140	53)	(141	14)	(142	24)
(145	42)	(146	18)	(149	13)	(155	266)	(156	429)
(157	135)	(158	132)	(159	23)	(160	40)	(162	9)
(171	8)	(172	31)	(173	617)	(174	88)	(175	39)
(185	10)	(186	22)	(187	13)	(199	8)	(202	14)
(223	8)	(229	74)	(236	10)	(254	8)	(255	13)
(261	10)	(262	8)	(268	8)	(275	23)	(276	13)
(285	7)								

NAME:12C_1747.3_1313EC36_[612; 4-Aminobutyric acid (2TBS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:175003-10-1

RI:1747

RT:10.670

NUM PEAKS: 19

(73	1000)	(74	93)	(75	182)	(78	34)	(84	207)
(100	39)	(112	314)	(115	34)	(129	51)	(131	27)
(133	53)	(147	369)	(148	60)	(149	43)	(156	48)
(184	29)	(194	48)	(274	267)	(275	59)		

NAME:12C_1784.4_1313EC36_Glutamine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:178001-10-1

RI:1785

RT:10.958

NUM PEAKS: 107

(70	19)	(71	11)	(72	44)	(73	1000)	(74	138)
(75	301)	(76	23)	(77	12)	(81	5)	(82	6)
(83	35)	(84	26)	(85	12)	(86	14)	(87	8)
(88	4)	(89	6)	(90	5)	(94	3)	(96	3)
(97	3)	(98	11)	(99	7)	(100	63)	(101	14)
(102	11)	(105	3)	(110	3)	(112	17)	(113	11)
(114	44)	(115	41)	(116	37)	(117	16)	(118	4)
(119	5)	(126	13)	(127	4)	(128	77)	(129	23)
(130	26)	(131	72)	(132	26)	(133	52)	(134	9)
(135	5)	(139	50)	(140	22)	(141	7)	(142	22)
(143	5)	(144	8)	(145	36)	(146	10)	(147	163)
(148	32)	(149	34)	(150	5)	(151	3)	(153	3)
(154	4)	(155	244)	(156	775)	(157	121)	(158	37)
(159	5)	(160	3)	(167	3)	(172	8)	(173	9)
(174	5)	(183	3)	(188	15)	(189	5)	(190	3)
(200	3)	(202	3)	(203	64)	(204	16)	(205	6)
(211	3)	(213	3)	(214	3)	(216	8)	(218	17)
(219	5)	(221	4)	(227	7)	(228	5)	(229	27)
(230	16)	(231	5)	(232	10)	(244	6)	(245	97)
(246	22)	(247	8)	(257	6)	(258	3)	(272	5)
(273	7)	(274	3)	(301	7)	(302	3)	(347	16)
(348	5)	(362	6)						

NAME:12C_1843.5_1313EC36_[919; D-Xylopyranose (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184004-10-1

140

RI:1844

RT:11.416

NUM PEAKS: 29

(72	19)	(73	1000)	(74	85)	(75	114)	(76	7)
(89	12)	(101	32)	(103	63)	(117	53)	(129	54)
(131	28)	(133	58)	(134	8)	(143	20)	(147	218)
(148	33)	(149	27)	(189	35)	(191	248)	(192	42)
(193	18)	(203	9)	(204	332)	(205	69)	(206	24)
(217	125)	(218	28)	(219	13)	(305	7)		

NAME:12C_1858.1_1313EC36_Lysine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1858 |RI:1858 |RI:1858

CASNO:186002-10-1

RI:1858

RT:11.530

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 99

(70	22)	(71	11)	(72	24)	(73	1000)	(74	161)
(75	194)	(76	18)	(77	8)	(80	6)	(81	3)
(82	59)	(83	11)	(84	200)	(85	25)	(86	214)
(87	28)	(88	41)	(89	6)	(90	3)	(94	14)
(95	3)	(97	6)	(98	12)	(99	11)	(100	120)
(101	22)	(102	40)	(103	19)	(104	4)	(110	7)
(111	3)	(112	24)	(113	10)	(114	39)	(115	17)
(116	20)	(117	24)	(118	6)	(119	4)	(126	7)
(127	3)	(128	56)	(129	15)	(130	71)	(131	34)
(132	21)	(133	21)	(134	4)	(140	10)	(141	3)
(142	27)	(143	7)	(144	15)	(145	4)	(146	35)
(147	67)	(148	20)	(149	8)	(154	7)	(155	5)
(156	177)	(157	28)	(158	20)	(159	4)	(160	7)
(161	3)	(162	4)	(166	4)	(167	7)	(168	39)
(169	6)	(170	5)	(172	19)	(173	5)	(174	916)
(175	169)	(176	74)	(177	8)	(183	4)	(184	8)
(186	15)	(187	4)	(188	4)	(199	3)	(200	191)
(201	35)	(202	12)	(216	7)	(230	23)	(231	6)
(232	3)	(257	4)	(258	46)	(259	10)	(260	4)
(289	6)	(347	3)	(362	16)	(363	6)		

NAME:12C_1888.7_1313EC36_[772; D-Glucose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189005-10-1

RI:1889

RT:11.768

NUM PEAKS: 6

(169	14)	(191	549)	(192	88)	(193	40)	(204	1000)
(398	3)								

NAME:12C_1892.7_1313EC36_Tyrosine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189006-10-1

RI:1893

RT:11.798

NUM PEAKS: 47

(75	399)	(76	36)	(77	44)	(78	21)	(79	15)
(80	5)	(82	63)	(87	36)	(90	52)	(91	83)
(92	10)	(93	6)	(95	8)	(107	14)	(109	5)
(118	34)	(119	58)	(120	7)	(121	8)	(123	3)
(135	43)	(136	5)	(137	5)	(146	71)	(150	8)
(151	20)	(163	41)	(164	19)	(165	34)	(166	8)
(175	12)	(176	15)	(177	16)	(178	16)	(179	1000)

141

(180 231) (181 57) (208 104) (209 21) (219 75)
 (220 11) (265 5) (282 3) (293 6) (310 29)
 (311 7) (312 3)

NAME:12C_1973.7_1313EC36_[945; beta-D-Glucopyranose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:197002-10-1

RI:1974

RT:12.324

NUM PEAKS: 66

(73 1000) (74 83) (75 95) (76 5) (77 5)
 (81 7) (83 3) (87 7) (88 4) (89 14)
 (101 30) (102 5) (103 64) (104 5) (105 4)
 (111 4) (113 3) (115 6) (116 14) (117 37)
 (118 4) (119 6) (129 64) (130 8) (131 28)
 (132 4) (133 56) (134 7) (135 5) (143 16)
 (145 5) (147 223) (148 35) (155 4) (157 8)
 (159 3) (161 3) (163 4) (169 9) (175 4)
 (177 3) (189 38) (190 11) (191 266) (192 47)
 (193 20) (203 12) (204 430) (205 84) (206 36)
 (207 8) (217 83) (218 23) (219 9) (221 7)
 (230 3) (231 9) (232 3) (233 3) (243 7)
 (291 6) (305 6) (317 3) (319 3) (345 3)
 (435 3)

NAME:12C_1924.5_1313EC16_Histidine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192006-10-1

RI:1925

RT:12.015

NUM PEAKS: 83

(70 10) (71 5) (72 23) (73 1000) (74 88)
 (75 87) (76 5) (81 43) (82 43) (83 17)
 (84 18) (90 7) (96 6) (97 4) (98 8)
 (104 34) (110 8) (111 6) (118 3) (119 25)
 (120 3) (125 4) (126 10) (132 35) (133 21)
 (134 4) (135 4) (137 3) (139 8) (147 95)
 (148 15) (149 8) (150 6) (151 3) (153 47)
 (154 1000) (155 214) (161 12) (165 3) (166 22)
 (167 8) (180 3) (181 3) (182 14) (183 5)
 (184 3) (191 9) (192 9) (193 3) (203 4)
 (206 11) (207 30) (208 7) (209 3) (211 3)
 (218 40) (219 8) (220 35) (222 3) (225 3)
 (226 14) (227 4) (233 3) (235 4) (238 36)
 (239 11) (240 4) (253 5) (254 171) (255 41)
 (256 16) (257 10) (266 8) (310 4) (322 3)
 (323 25) (324 7) (325 3) (328 5) (336 4)
 (356 13) (357 5) (371 5)

NAME:12C_2091.2_1313EC11_myo-Inositol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209002-10-1

RI:2091

RT:13.074

NUM PEAKS: 112

(72 16) (73 1000) (74 86) (75 67) (76 3)
 (81 9) (83 3) (85 3) (87 6) (97 3)
 (99 6) (100 3) (103 57) (108 3) (111 8)
 (113 6) (115 7) (116 7) (117 8) (125 3)
 (127 4) (129 76) (130 11) (131 32) (133 74)

142

(134	11)	(135	6)	(141	4)	(142	3)	(143	23)
(144	6)	(147	319)	(148	50)	(149	20)	(154	3)
(155	4)	(156	4)	(157	7)	(159	4)	(167	3)
(169	4)	(175	13)	(177	7)	(189	15)	(190	13)
(191	103)	(192	24)	(193	10)	(195	3)	(201	4)
(203	7)	(204	43)	(205	15)	(215	4)	(216	5)
(217	168)	(218	35)	(219	17)	(230	7)	(231	5)
(242	3)	(243	7)	(244	3)	(245	3)	(254	3)
(260	3)	(265	27)	(266	9)	(267	5)	(291	15)
(292	6)	(293	6)	(304	11)	(305	98)	(306	32)
(307	18)	(308	6)	(317	8)	(318	55)	(319	25)
(320	11)	(321	4)	(331	3)	(343	3)	(344	3)
(345	3)	(353	3)	(365	3)	(367	7)	(368	5)
(369	3)	(379	3)	(391	3)	(392	3)	(393	5)
(394	3)	(398	3)	(403	3)	(408	3)	(417	3)
(421	3)	(430	3)	(431	3)	(432	10)	(433	8)
(434	6)	(435	3)	(444	3)	(454	3)	(506	3)
(507	5)	(508	3)						

NAME:12C_1293.1_1313EC75_Glycerol (3TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:129003-10-1
 RI:1293
 RT:6.323

NUM PEAKS: 58

(70	4)	(71	8)	(72	25)	(73	1000)	(74	91)
(75	90)	(76	5)	(85	9)	(87	13)	(88	13)
(89	47)	(90	5)	(99	6)	(101	72)	(102	11)
(103	321)	(104	33)	(105	21)	(113	7)	(116	27)
(117	321)	(118	34)	(119	33)	(120	3)	(129	66)
(130	10)	(131	58)	(132	10)	(133	231)	(134	34)
(145	3)	(147	583)	(148	92)	(149	64)	(150	8)
(159	5)	(161	3)	(163	12)	(174	4)	(175	56)
(176	11)	(177	33)	(178	7)	(189	10)	(190	3)
(191	36)	(192	7)	(203	29)	(204	43)	(205	268)
(206	56)	(207	29)	(217	17)	(218	113)	(219	25)
(220	11)	(221	5)	(293	10)				

NAME:12C_1317.6_1313EC75_Threonine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:132001-10-1
 RI:1318

RT:6.611

NUM PEAKS: 51

(71	11)	(72	29)	(73	1000)	(74	129)	(75	300)
(76	25)	(77	17)	(81	5)	(85	8)	(86	8)
(87	49)	(88	10)	(89	7)	(91	3)	(98	9)
(100	8)	(101	31)	(102	18)	(103	12)	(104	6)
(105	5)	(112	3)	(114	19)	(115	25)	(116	18)
(117	273)	(118	31)	(119	15)	(128	3)	(129	6)
(130	206)	(131	83)	(132	59)	(133	36)	(134	8)
(135	4)	(145	3)	(146	73)	(147	172)	(148	35)
(149	15)	(150	3)	(176	3)	(177	3)	(181	4)
(203	3)	(204	8)	(219	76)	(220	20)	(221	8)
(248	8)								

NAME:12C_1318.4_1313EC75_Proline (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:132003-10-1
 RI:1318

143

RT:6.620

NUM PEAKS: 32

(70	47)	(71	10)	(72	46)	(73	608)	(80	5)
(83	3)	(84	13)	(85	7)	(86	6)	(96	3)
(97	3)	(98	7)	(99	12)	(100	12)	(103	9)
(113	7)	(124	4)	(126	4)	(127	5)	(128	3)
(140	12)	(141	8)	(142	1000)	(143	137)	(144	39)
(145	3)	(147	80)	(170	10)	(175	5)	(216	44)
(217	9)	(244	5)						

NAME:12C_1338.0_1313EC75_Succinic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:134001-10-1

RI:1338

RT:6.850

NUM PEAKS: 32

(72	29)	(73	547)	(75	415)	(79	4)	(86	13)
(87	9)	(89	10)	(101	9)	(102	4)	(113	6)
(115	12)	(116	18)	(117	14)	(129	95)	(130	4)
(131	23)	(133	46)	(143	5)	(145	5)	(147	1000)
(148	154)	(157	4)	(163	3)	(172	44)	(173	22)
(174	4)	(175	14)	(218	6)	(247	79)	(248	16)
(249	7)	(262	3)						

NAME:12C_1378.1_1313EC75_Alanine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138002-10-1

RI:1378

RT:7.321

NUM PEAKS: 54

(70	24)	(71	10)	(72	28)	(73	1000)	(74	79)
(84	3)	(85	7)	(86	12)	(87	8)	(98	3)
(99	5)	(100	616)	(101	68)	(102	26)	(113	8)
(114	158)	(115	32)	(116	26)	(117	26)	(118	4)
(119	11)	(131	46)	(132	9)	(133	154)	(134	21)
(135	11)	(142	3)	(147	220)	(148	33)	(149	16)
(158	14)	(159	3)	(160	5)	(161	3)	(172	24)
(173	3)	(174	14)	(175	11)	(187	3)	(188	726)
(189	138)	(190	57)	(191	18)	(192	3)	(200	3)
(202	15)	(203	3)	(246	4)	(261	3)	(262	97)
(263	29)	(264	13)	(290	18)	(291	6)		

NAME:12C_1381.0_1313EC75_Serine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:138001-10-1

RI:1381

RT:7.354

NUM PEAKS: 31

(72	31)	(73	1000)	(74	96)	(86	18)	(88	19)
(102	16)	(116	71)	(118	8)	(119	8)	(135	6)
(147	138)	(148	26)	(149	19)	(160	5)	(163	7)
(174	15)	(203	11)	(204	348)	(205	68)	(206	27)
(207	4)	(216	13)	(217	6)	(218	178)	(219	36)
(220	16)	(221	5)	(278	18)	(279	7)	(306	9)
(307	4)								

NAME:12C_1410.5_1313EC75_[700; 2-methyl-1,2-propanediol (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:141003-10-1

RI:1411

144

RT:7.700

NUM PEAKS: 33

(73 1000)	(102 98)	(104 4)	(115 46)	(119 8)
(131 688)	(132 83)	(133 109)	(134 13)	(135 8)
(143 36)	(144 7)	(145 8)	(147 202)	(149 44)
(150 5)	(161 4)	(189 3)	(191 14)	(203 6)
(204 7)	(207 4)	(217 6)	(220 5)	(221 24)
(222 6)	(223 3)	(277 10)	(291 7)	(292 89)
(293 26)	(294 12)	(335 4)		

NAME:12C_1419.8_1313EC75_Alanine {BP} (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:142001-10-1

RI:1420

RT:7.810

NUM PEAKS: 38

(70 150)	(72 50)	(73 1000)	(74 101)	(75 344)
(76 22)	(86 38)	(94 11)	(100 148)	(101 24)
(102 20)	(115 12)	(116 491)	(117 82)	(118 21)
(119 6)	(131 14)	(133 51)	(144 43)	(145 12)
(147 332)	(148 50)	(149 38)	(160 455)	(161 52)
(162 16)	(175 7)	(187 5)	(190 128)	(191 22)
(192 9)	(218 9)	(233 11)	(234 19)	(255 8)
(262 74)	(263 14)	(264 5)		

NAME:12C_1464.2_1313EC75_[725; 2-Ketooctanoic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:146003-10-1

RI:1464

RT:8.330

NUM PEAKS: 82

(70 6)	(71 8)	(72 26)	(73 674)	(74 64)
(75 249)	(76 17)	(77 24)	(79 8)	(80 3)
(81 39)	(82 4)	(83 38)	(84 7)	(85 12)
(86 3)	(87 8)	(89 4)	(93 4)	(94 12)
(95 51)	(96 61)	(97 16)	(98 7)	(99 13)
(100 6)	(101 5)	(102 3)	(103 8)	(105 4)
(109 9)	(110 4)	(111 17)	(112 5)	(113 3)
(115 8)	(116 3)	(117 11)	(119 5)	(122 18)
(123 4)	(124 4)	(125 21)	(126 10)	(127 7)
(131 20)	(132 4)	(133 60)	(134 8)	(135 6)
(136 9)	(140 11)	(141 7)	(143 4)	(147 1000)
(148 161)	(149 97)	(150 10)	(151 3)	(153 7)
(155 6)	(157 12)	(168 10)	(169 30)	(170 7)
(171 4)	(184 10)	(185 37)	(186 6)	(196 3)
(197 5)	(212 73)	(213 22)	(214 5)	(215 5)
(258 3)	(259 9)	(286 4)	(287 81)	(288 19)
(289 7)	(302 2)			

NAME:12C_1520.6_1313EC75_Aspartic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152002-10-1

RI:1521

RT:8.910

NUM PEAKS: 73

(70 42)	(71 9)	(72 31)	(73 1000)	(74 107)
(75 167)	(77 8)	(83 4)	(85 5)	(86 11)
(87 6)	(88 3)	(89 4)	(98 10)	(100 253)
(101 32)	(102 17)	(105 3)	(114 5)	(115 17)
(116 11)	(117 62)	(118 7)	(119 12)	(129 5)

145

(130	29)	(131	23)	(132	19)	(133	56)	(134	10)
(135	6)	(142	17)	(143	7)	(144	9)	(145	3)
(146	5)	(147	167)	(148	29)	(149	27)	(150	3)
(158	3)	(160	9)	(161	3)	(163	17)	(164	3)
(172	9)	(173	3)	(174	14)	(175	3)	(177	4)
(188	45)	(189	11)	(190	7)	(202	46)	(203	9)
(204	13)	(205	4)	(216	21)	(217	7)	(218	80)
(220	6)	(221	4)	(231	6)	(232	382)	(233	80)
(234	38)	(244	4)	(245	4)	(246	3)	(292	5)
(306	11)	(307	3)	(334	5)				

NAME:12C_1529.0_1313EC75_Pyroglutamic acid (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:153002-10-1

RI:1529

RT:8.976

NUM PEAKS: 63

(70	20)	(71	11)	(72	45)	(73	883)	(74	81)
(75	125)	(76	8)	(80	4)	(82	6)	(83	7)
(84	28)	(85	18)	(86	24)	(87	9)	(88	3)
(89	3)	(94	3)	(96	3)	(97	3)	(98	7)
(99	9)	(100	17)	(101	5)	(102	5)	(103	8)
(105	3)	(110	5)	(112	25)	(113	8)	(114	14)
(115	8)	(117	10)	(119	3)	(122	3)	(126	3)
(129	4)	(131	19)	(132	5)	(133	35)	(134	5)
(135	3)	(140	28)	(141	10)	(142	8)	(147	160)
(148	26)	(149	16)	(154	9)	(155	6)	(156	1000)
(157	130)	(158	43)	(174	3)	(214	12)	(215	3)
(228	3)	(230	84)	(231	19)	(232	7)	(258	76)
(259	17)	(260	7)	(273	3)				

NAME:12C_1659.6_1313EC75_[910; 2-Ketogluconic acid methoxyamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:166002-10-1

RI:1660

RT:9.991

NUM PEAKS: 40

(72	21)	(73	1000)	(74	79)	(75	73)	(84	21)
(87	8)	(89	26)	(101	34)	(103	168)	(104	14)
(115	8)	(116	13)	(117	120)	(118	11)	(119	9)
(129	42)	(131	44)	(133	71)	(143	8)	(147	258)
(148	37)	(149	24)	(157	11)	(158	7)	(172	35)
(175	10)	(189	57)	(190	11)	(201	91)	(202	16)
(203	14)	(204	275)	(205	107)	(206	30)	(217	82)
(242	5)	(256	12)	(288	8)	(291	16)	(302	6)

NAME:12C_1755.7_1313EC75_[829; Orotic acid (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176003-10-1

RI:1756

RT:10.739

NUM PEAKS: 94

(72	85)	(73	1000)	(78	4)	(79	12)	(80	8)
(81	8)	(83	17)	(86	48)	(91	8)	(92	4)
(93	9)	(94	7)	(97	21)	(100	165)	(102	9)
(104	3)	(105	7)	(106	5)	(107	4)	(108	3)
(109	3)	(119	8)	(120	5)	(123	6)	(124	4)
(131	66)	(132	15)	(133	66)	(134	10)	(135	7)
(137	4)	(147	214)	(148	35)	(149	20)	(156	10)
(158	15)	(160	9)	(161	5)	(167	9)	(174	77)

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(175	12)	(176	6)	(181	8)	(182	3)	(188	4)
(189	8)	(190	10)	(191	16)	(192	5)	(195	8)
(213	5)	(214	13)	(215	5)	(225	7)	(226	7)
(227	3)	(228	3)	(239	24)	(240	7)	(241	5)
(245	3)	(252	6)	(253	74)	(254	502)	(255	127)
(256	44)	(257	5)	(268	4)	(269	60)	(270	27)
(271	7)	(272	3)	(282	11)	(283	5)	(285	3)
(299	4)	(305	8)	(306	8)	(313	3)	(327	4)
(328	3)	(329	8)	(330	3)	(333	7)	(341	3)
(343	4)	(344	4)	(356	22)	(357	131)	(358	40)
(359	16)	(371	8)	(372	12)	(373	4)		

NAME:12C_1758.1_1313EC75_[636; 4R-Acetamido-2,3-(Z)-epoxy-4-(E)-hydroxycyclohexane (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176005-10-1

RI:1758

RT:10.757

NUM PEAKS: 89

(70	1000)	(71	97)	(72	22)	(73	525)	(74	109)
(75	231)	(76	21)	(77	8)	(80	3)	(82	5)
(83	20)	(84	97)	(85	186)	(86	26)	(87	17)
(88	6)	(90	23)	(91	3)	(95	47)	(96	15)
(97	8)	(98	31)	(99	122)	(100	32)	(101	21)
(102	10)	(103	26)	(104	3)	(110	5)	(111	5)
(112	9)	(113	18)	(114	14)	(115	27)	(116	28)
(117	20)	(118	4)	(122	5)	(124	3)	(125	30)
(126	18)	(127	37)	(128	10)	(129	25)	(130	53)
(131	27)	(132	10)	(139	9)	(140	24)	(141	54)
(143	15)	(144	20)	(145	7)	(146	7)	(147	30)
(148	6)	(149	5)	(151	3)	(152	4)	(154	8)
(155	13)	(156	5)	(157	19)	(158	5)	(159	27)
(160	4)	(167	9)	(168	39)	(169	12)	(170	10)
(171	10)	(172	82)	(173	16)	(183	18)	(184	416)
(185	65)	(186	55)	(187	21)	(188	4)	(196	5)
(211	9)	(212	3)	(229	4)	(258	11)	(259	3)
(284	3)	(285	3)	(286	8)	(301	3)		

NAME:12C_1763.9_1313EC75_Ornithine (3TMS); Arginine (BP) (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176006-10-1

RI:1764

RT:10.803

NUM PEAKS: 96

(70	139)	(71	16)	(72	26)	(73	1000)	(74	173)
(75	186)	(76	17)	(77	7)	(80	9)	(82	3)
(83	5)	(84	9)	(85	10)	(86	210)	(87	38)
(88	14)	(90	15)	(91	3)	(96	9)	(97	17)
(98	15)	(99	10)	(100	115)	(101	18)	(102	36)
(103	13)	(104	4)	(110	5)	(112	10)	(113	10)
(114	20)	(115	19)	(116	22)	(117	24)	(118	5)
(119	3)	(126	7)	(128	43)	(129	11)	(130	75)
(131	48)	(132	27)	(133	17)	(134	4)	(140	7)
(141	7)	(142	188)	(143	30)	(144	28)	(145	5)
(146	60)	(147	94)	(148	31)	(149	13)	(150	3)
(152	4)	(153	6)	(154	23)	(155	4)	(156	5)
(157	3)	(158	13)	(159	26)	(160	14)	(161	12)
(162	8)	(169	12)	(170	13)	(171	5)	(172	45)
(173	9)	(174	697)	(175	129)	(176	59)	(177	7)
(186	203)	(187	47)	(188	15)	(189	3)	(200	11)

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(201 3) (204 5) (213 3) (215 4) (216 33)
 (217 7) (218 4) (243 9) (244 62) (245 14)
 (246 5) (258 18) (259 7) (348 37) (349 12)
 (350 5)

NAME:12C_1769.9_1313EC75_Glycerol-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177002-10-1

RI:1770

RT:10.850

NUM PEAKS: 108

(71 7) (72 27) (73 1000) (74 86) (77 15)
 (85 7) (88 6) (91 5) (99 6) (101 102)
 (103 118) (104 12) (105 12) (107 5) (113 20)
 (115 23) (116 25) (117 24) (119 13) (121 7)
 (123 3) (129 69) (131 56) (132 8) (133 113)
 (134 15) (135 33) (136 4) (137 13) (139 3)
 (147 155) (148 23) (149 21) (150 3) (151 9)
 (153 3) (163 8) (165 4) (177 3) (179 4)
 (181 17) (182 3) (183 8) (191 16) (193 20)
 (194 4) (195 18) (196 3) (197 6) (203 11)
 (205 8) (207 32) (208 7) (209 6) (210 3)
 (211 93) (212 17) (213 11) (220 3) (225 20)
 (226 6) (227 18) (228 3) (241 17) (242 4)
 (243 10) (253 6) (255 4) (256 19) (269 6)
 (283 6) (284 3) (285 19) (286 5) (287 3)
 (298 18) (299 175) (300 47) (301 25) (302 5)
 (313 4) (314 11) (315 42) (316 12) (317 6)
 (327 4) (328 9) (341 14) (342 7) (343 3)
 (356 18) (357 112) (358 34) (359 16) (360 3)
 (369 3) (370 21) (371 7) (372 4) (373 9)
 (374 3) (386 3) (387 12) (388 5) (389 5)
 (444 4) (445 17) (446 7)

NAME:12C_1802.0_1313EC75_[706; Xylitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180002-10-1

RI:1802

RT:11.098

NUM PEAKS: 69

(72 14) (73 1000) (74 101) (75 140) (87 4)
 (88 4) (89 11) (100 4) (101 12) (102 11)
 (103 34) (104 6) (113 5) (115 6) (116 8)
 (117 40) (118 6) (119 5) (128 13) (129 50)
 (130 10) (131 19) (132 5) (133 35) (134 5)
 (135 4) (141 21) (142 6) (143 19) (144 10)
 (145 3) (147 141) (148 21) (149 19) (155 5)
 (157 23) (169 9) (189 20) (190 4) (191 33)
 (192 5) (203 3) (205 16) (206 3) (215 9)
 (217 54) (218 13) (219 11) (220 3) (221 7)
 (229 8) (230 6) (231 7) (232 4) (243 3)
 (245 3) (246 4) (257 39) (258 10) (259 4)
 (272 4) (303 6) (319 6) (347 5) (362 3)
 (436 5) (437 23) (438 11) (439 5)

NAME:12C_1813.0_1313EC75_Glyceric acid-3-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181003-10-1

RI:1813

RT:11.184

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NUM PEAKS: 69

(72	28)	(73	1000)	(74	80)	(75	112)	(77	20)
(87	9)	(89	17)	(90	5)	(101	87)	(102	11)
(104	7)	(105	13)	(107	6)	(115	16)	(116	29)
(117	17)	(121	10)	(132	8)	(133	101)	(134	16)
(135	32)	(137	15)	(141	4)	(144	6)	(147	252)
(148	39)	(149	26)	(151	11)	(153	5)	(181	19)
(189	15)	(190	5)	(193	19)	(194	5)	(195	18)
(207	28)	(211	118)	(212	20)	(213	12)	(214	5)
(225	19)	(226	7)	(227	99)	(228	17)	(229	9)
(243	5)	(298	12)	(299	125)	(300	36)	(301	17)
(302	3)	(315	45)	(316	14)	(317	8)	(341	11)
(342	6)	(343	6)	(352	3)	(356	14)	(357	66)
(358	20)	(359	8)	(386	10)	(387	32)	(388	14)
(389	8)	(458	6)	(459	13)	(460	6)		

NAME:12C_1819.8_1313EC75_Ornithine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182002-10-1

RI:1820

RT:11.237

NUM PEAKS: 105

(70	24)	(71	9)	(72	19)	(73	1000)	(74	117)
(80	3)	(82	3)	(83	4)	(84	12)	(85	10)
(86	112)	(87	16)	(88	7)	(90	5)	(91	3)
(96	5)	(98	14)	(100	104)	(101	18)	(102	46)
(103	19)	(104	4)	(110	9)	(112	17)	(113	9)
(114	31)	(115	23)	(116	16)	(117	19)	(118	5)
(119	6)	(124	3)	(126	19)	(127	13)	(128	53)
(130	59)	(131	31)	(132	29)	(133	26)	(134	6)
(140	12)	(141	12)	(142	898)	(143	127)	(144	49)
(145	6)	(146	41)	(152	7)	(153	4)	(154	6)
(156	4)	(158	9)	(159	6)	(160	12)	(161	5)
(162	4)	(168	4)	(169	10)	(170	6)	(172	38)
(173	9)	(174	294)	(175	54)	(176	29)	(177	4)
(186	13)	(187	12)	(188	9)	(189	15)	(190	5)
(191	7)	(198	3)	(200	57)	(201	14)	(202	10)
(203	8)	(204	19)	(205	5)	(214	30)	(215	10)
(216	33)	(217	12)	(218	17)	(219	4)	(220	5)
(226	3)	(230	4)	(232	4)	(241	6)	(242	4)
(243	3)	(244	6)	(258	21)	(259	21)	(260	6)
(303	4)	(315	5)	(316	3)	(330	7)	(331	3)
(405	3)	(419	3)	(420	15)	(421	7)	(422	4)

NAME:12C_1827.9_1313EC75_Arginine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:183001-10-1

RI:1828

RT:11.300

NUM PEAKS: 43

(70	162)	(71	26)	(73	1000)	(74	25)	(84	87)
(85	30)	(98	17)	(100	88)	(112	7)	(114	17)
(115	41)	(125	7)	(126	5)	(127	21)	(128	15)
(130	10)	(132	15)	(140	41)	(141	122)	(142	239)
(143	17)	(155	25)	(156	26)	(157	667)	(158	83)
(167	9)	(168	14)	(171	25)	(172	33)	(173	5)
(187	13)	(188	7)	(215	7)	(216	13)	(240	10)
(244	15)	(256	223)	(257	50)	(258	15)	(292	3)
(358	4)	(371	2)	(373	5)				

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NAME:12C_1835.3_1313EC75_[731; Erythrose (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184003-10-1

RI:1835

RT:11.358

NUM PEAKS: 137

(70	8)	(71	7)	(72	22)	(73	1000)	(74	89)
(75	143)	(76	9)	(77	11)	(80	4)	(81	3)
(82	6)	(83	37)	(84	87)	(85	15)	(86	5)
(87	12)	(88	6)	(89	43)	(90	4)	(91	3)
(94	3)	(96	12)	(97	4)	(98	4)	(99	15)
(100	21)	(101	33)	(102	9)	(103	93)	(104	10)
(108	6)	(109	3)	(110	3)	(111	10)	(112	4)
(113	26)	(114	11)	(115	25)	(116	32)	(117	131)
(118	14)	(119	14)	(122	3)	(124	3)	(126	3)
(127	5)	(128	20)	(129	84)	(130	18)	(131	42)
(132	10)	(133	74)	(134	11)	(135	10)	(136	6)
(141	4)	(142	7)	(143	22)	(144	13)	(145	7)
(146	3)	(147	250)	(148	40)	(149	47)	(150	10)
(151	3)	(152	3)	(155	4)	(156	45)	(157	22)
(158	12)	(159	27)	(163	20)	(164	4)	(168	12)
(173	29)	(174	8)	(175	7)	(177	10)	(182	11)
(183	4)	(184	12)	(185	4)	(186	4)	(189	45)
(190	11)	(191	75)	(192	13)	(193	6)	(196	7)
(197	5)	(198	23)	(199	4)	(200	3)	(201	5)
(202	17)	(203	42)	(204	68)	(205	21)	(206	7)
(207	3)	(210	9)	(211	6)	(215	8)	(216	4)
(217	103)	(218	89)	(219	23)	(220	7)	(221	3)
(224	7)	(226	54)	(227	9)	(228	3)	(229	3)
(230	10)	(231	43)	(232	11)	(233	24)	(234	5)
(239	6)	(240	3)	(245	3)	(246	8)	(258	4)
(272	5)	(300	10)	(301	3)	(314	5)	(316	7)
(317	3)	(318	10)	(319	6)	(320	3)	(329	24)
(330	7)	(404	5)						

NAME:12C_1869.1_1313EC75_Fructose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187002-10-1

RI:1869

RT:11.621

NUM PEAKS: 87

(70	5)	(71	5)	(72	19)	(73	1000)	(74	83)
(75	63)	(76	3)	(82	4)	(84	16)	(85	5)
(87	7)	(88	6)	(89	47)	(90	4)	(99	4)
(100	10)	(101	17)	(102	5)	(103	351)	(104	35)
(105	17)	(113	4)	(114	8)	(115	7)	(116	5)
(117	54)	(118	6)	(119	8)	(126	3)	(128	3)
(129	40)	(130	8)	(131	22)	(132	4)	(133	71)
(134	9)	(135	5)	(142	5)	(143	8)	(145	5)
(147	183)	(148	30)	(149	19)	(157	7)	(158	3)
(159	3)	(163	8)	(172	14)	(173	17)	(174	4)
(175	6)	(177	4)	(189	30)	(190	7)	(191	16)
(192	3)	(201	8)	(202	6)	(203	4)	(204	14)
(205	22)	(206	5)	(207	5)	(214	3)	(216	5)
(217	222)	(218	46)	(219	22)	(220	3)	(221	6)
(231	6)	(244	3)	(256	3)	(260	3)	(262	4)
(263	6)	(277	17)	(278	6)	(279	3)	(291	4)
(306	3)	(307	76)	(308	23)	(309	11)	(335	5)
(364	11)	(365	4)						

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NAME:12C_1879.6_1313EC75_Fructose methoxyamine (BP) (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188004-10-1

RI:1880

RT:11.703

NUM PEAKS: 81

(70	6)	(71	5)	(72	19)	(73	1000)	(74	88)
(75	78)	(82	7)	(84	35)	(85	7)	(86	4)
(87	8)	(88	6)	(89	72)	(90	6)	(99	4)
(100	12)	(101	21)	(102	5)	(103	365)	(104	38)
(105	26)	(113	6)	(114	26)	(115	9)	(116	8)
(117	55)	(118	7)	(119	11)	(126	3)	(128	4)
(129	40)	(133	59)	(134	8)	(135	5)	(142	7)
(143	9)	(145	6)	(147	216)	(148	35)	(156	3)
(159	3)	(172	9)	(173	17)	(175	7)	(177	3)
(188	3)	(189	29)	(190	7)	(191	18)	(192	3)
(198	3)	(201	7)	(202	8)	(203	5)	(204	16)
(205	28)	(206	6)	(207	5)	(216	5)	(217	255)
(218	55)	(219	25)	(221	7)	(231	6)	(244	6)
(245	3)	(262	14)	(263	9)	(264	3)	(277	18)
(278	6)	(279	3)	(291	3)	(306	4)	(307	86)
(308	26)	(309	12)	(335	5)	(336	3)	(364	12)
(365	4)								

NAME:12C_1931.9_1313EC75_Sorbitol (6TMS); Glucitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193001-10-1

RI:1932

RT:12.063

NUM PEAKS: 90

(70	3)	(71	4)	(72	19)	(73	1000)	(74	88)
(75	66)	(76	3)	(81	3)	(83	10)	(85	4)
(87	8)	(88	5)	(89	26)	(90	3)	(97	6)
(99	4)	(101	24)	(102	5)	(103	175)	(104	17)
(105	9)	(111	3)	(113	5)	(115	7)	(116	7)
(117	100)	(118	10)	(119	8)	(127	3)	(129	83)
(130	10)	(131	27)	(132	4)	(133	59)	(134	8)
(135	6)	(141	3)	(143	14)	(145	4)	(147	316)
(148	51)	(149	33)	(150	4)	(155	4)	(157	60)
(158	8)	(159	5)	(163	5)	(169	4)	(175	9)
(177	5)	(183	7)	(189	34)	(190	9)	(191	32)
(192	6)	(193	3)	(203	5)	(204	41)	(205	148)
(206	30)	(207	15)	(217	153)	(218	32)	(219	14)
(220	3)	(221	9)	(229	15)	(230	6)	(231	16)
(232	4)	(255	6)	(259	4)	(277	7)	(278	4)
(291	7)	(305	8)	(306	5)	(307	24)	(308	7)
(309	3)	(318	7)	(319	118)	(320	38)	(321	17)
(322	4)	(331	8)	(332	3)	(345	5)	(421	3)

NAME:12C_1956.6_1313EC75_[793; D-Galactono-1,4-lactone (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:196004-10-1

RI:1957

RT:12.219

NUM PEAKS: 124

(70	11)	(71	5)	(72	20)	(73	1000)	(74	85)
(75	117)	(76	10)	(77	8)	(81	12)	(82	17)
(83	5)	(85	6)	(86	4)	(87	7)	(88	5)
(89	50)	(90	5)	(91	6)	(96	3)	(97	4)
(98	3)	(99	7)	(100	11)	(101	24)	(102	11)

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(103	101)	(104	11)	(105	14)	(109	5)	(110	5)
(111	7)	(112	3)	(113	5)	(114	5)	(115	11)
(116	11)	(117	54)	(118	7)	(119	10)	(126	4)
(127	5)	(128	5)	(129	88)	(130	30)	(131	31)
(132	7)	(133	56)	(134	8)	(135	6)	(139	3)
(141	3)	(142	12)	(143	18)	(144	5)	(145	8)
(146	4)	(147	165)	(148	48)	(149	26)	(150	4)
(153	4)	(154	3)	(155	12)	(156	4)	(157	29)
(158	12)	(159	5)	(160	15)	(161	14)	(162	3)
(163	10)	(168	4)	(169	55)	(170	34)	(171	9)
(172	4)	(173	4)	(174	8)	(177	3)	(183	4)
(186	9)	(189	34)	(190	8)	(191	21)	(192	4)
(200	3)	(201	3)	(203	7)	(204	48)	(205	21)
(206	6)	(207	3)	(215	4)	(216	5)	(217	218)
(218	47)	(219	31)	(220	5)	(221	4)	(228	3)
(229	7)	(230	4)	(231	6)	(232	3)	(242	6)
(243	28)	(244	13)	(245	8)	(246	4)	(247	4)
(248	3)	(259	3)	(260	4)	(271	18)	(272	5)
(273	3)	(291	3)	(331	5)	(332	13)	(333	5)
(360	4)	(361	43)	(362	15)	(363	7)		

NAME:12C_1999.3_1313EC75_Gluconic acid (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200001-10-1

RI:1999

RT:12.490

NUM PEAKS: 87

(72	18)	(73	1000)	(74	88)	(75	67)	(76	3)
(81	7)	(82	8)	(83	28)	(84	8)	(85	10)
(89	14)	(96	5)	(97	26)	(98	5)	(101	15)
(102	14)	(103	98)	(104	9)	(105	6)	(111	12)
(113	4)	(115	4)	(117	56)	(118	6)	(119	7)
(125	6)	(129	48)	(130	12)	(131	27)	(132	4)
(133	53)	(134	7)	(135	6)	(143	30)	(144	3)
(145	3)	(147	310)	(148	49)	(149	31)	(150	3)
(153	3)	(157	19)	(161	3)	(169	5)	(171	6)
(175	5)	(189	32)	(190	9)	(191	18)	(204	32)
(205	58)	(206	12)	(207	10)	(217	66)	(218	14)
(219	12)	(220	4)	(221	14)	(222	3)	(229	7)
(230	3)	(231	4)	(245	5)	(277	10)	(278	3)
(291	8)	(292	59)	(293	18)	(294	8)	(305	25)
(306	9)	(307	8)	(318	3)	(319	27)	(320	9)
(331	4)	(332	7)	(333	55)	(334	18)	(335	8)
(345	3)	(359	8)	(360	3)	(423	6)	(433	3)
(434	3)	(435	4)						

NAME:12C_2048.2_1313EC75_Hexadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:205001-10-1

RI:2048

RT:12.799

NUM PEAKS: 111

(70	27)	(71	43)	(72	51)	(73	944)	(74	111)
(75	1000)	(76	74)	(77	54)	(79	26)	(80	4)
(81	70)	(82	10)	(83	74)	(84	29)	(85	30)
(86	14)	(87	11)	(88	8)	(89	29)	(90	5)
(91	11)	(93	23)	(94	4)	(95	65)	(96	10)
(97	54)	(98	41)	(99	27)	(100	5)	(101	17)
(102	6)	(105	29)	(106	3)	(107	12)	(109	19)
(110	4)	(111	25)	(112	12)	(113	6)	(115	10)

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(116	67)	(117	969)	(118	95)	(119	41)	(121	9)
(123	6)	(125	7)	(126	5)	(127	5)	(128	4)
(129	492)	(130	64)	(131	174)	(132	459)	(133	90)
(134	22)	(135	9)	(137	3)	(139	5)	(140	5)
(141	4)	(142	4)	(143	45)	(144	7)	(145	233)
(146	31)	(153	5)	(154	7)	(155	6)	(157	15)
(158	4)	(159	26)	(167	3)	(168	3)	(171	24)
(172	4)	(173	8)	(174	6)	(185	33)	(186	5)
(187	21)	(188	6)	(195	4)	(199	10)	(201	53)
(202	10)	(203	3)	(213	10)	(214	3)	(215	8)
(216	3)	(227	11)	(228	3)	(229	12)	(230	3)
(241	5)	(243	12)	(244	3)	(257	7)	(269	15)
(270	4)	(271	4)	(283	3)	(285	15)	(286	4)
(312	15)	(313	233)	(314	66)	(315	17)	(328	26)
(329	8)								

NAME:12C_2087.4_1313EC75_[756; beta-D-Methylglucopyranoside (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:209004-10-1

RI:2087

RT:13.047

NUM PEAKS: 68

(70	6)	(72	21)	(73	1000)	(74	88)	(75	70)
(81	6)	(82	6)	(83	7)	(86	6)	(88	3)
(89	78)	(90	7)	(97	4)	(100	42)	(101	34)
(102	16)	(103	61)	(105	11)	(115	8)	(116	15)
(117	36)	(118	4)	(129	57)	(130	10)	(131	27)
(132	12)	(133	44)	(134	7)	(135	6)	(142	5)
(143	13)	(145	7)	(147	212)	(148	60)	(149	28)
(155	5)	(157	30)	(160	9)	(161	5)	(163	8)
(169	8)	(172	10)	(187	3)	(189	31)	(190	9)
(201	5)	(203	12)	(204	342)	(205	83)	(206	32)
(207	8)	(216	3)	(217	56)	(218	16)	(219	8)
(220	69)	(221	18)	(222	6)	(229	6)	(230	5)
(231	8)	(233	10)	(243	8)	(244	5)	(247	3)
(319	64)	(320	23)	(321	11)				

NAME:12C_2064.0_1191EC10_[770; 3,4,6-Trishydroxyphenylethanolamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:206001-10-1

RI:2064

RT:13.339

NUM PEAKS: 191

(70	28)	(71	17)	(72	20)	(75	211)	(77	38)
(81	37)	(82	17)	(83	13)	(86	301)	(87	27)
(88	5)	(90	3)	(91	11)	(93	24)	(95	10)
(96	4)	(98	7)	(100	150)	(101	32)	(102	84)
(105	5)	(106	4)	(107	6)	(109	20)	(112	6)
(113	9)	(114	12)	(115	15)	(116	15)	(117	181)
(118	16)	(119	11)	(121	7)	(122	4)	(123	14)
(124	3)	(125	9)	(128	8)	(130	62)	(131	20)
(132	25)	(133	44)	(134	5)	(135	6)	(136	7)
(137	4)	(139	4)	(142	13)	(143	10)	(144	13)
(146	19)	(147	61)	(148	15)	(149	16)	(150	4)
(151	4)	(156	5)	(157	7)	(158	34)	(161	3)
(162	6)	(164	5)	(170	6)	(171	12)	(172	37)
(173	5)	(174	1000)	(175	168)	(176	129)	(177	15)
(182	6)	(186	8)	(187	14)	(188	10)	(189	6)
(191	11)	(196	5)	(199	6)	(200	9)	(201	5)
(202	8)	(203	4)	(204	16)	(207	9)	(208	7)

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(211	8)	(213	5)	(217	8)	(220	8)	(226	4)
(227	13)	(233	7)	(234	3)	(235	3)	(243	6)
(244	4)	(246	3)	(248	8)	(250	3)	(252	9)
(257	13)	(258	8)	(259	9)	(261	6)	(262	3)
(264	8)	(266	11)	(269	6)	(270	3)	(271	3)
(275	8)	(276	6)	(284	5)	(285	7)	(290	3)
(291	3)	(301	3)	(303	5)	(307	3)	(309	4)
(310	4)	(311	3)	(313	5)	(317	5)	(321	7)
(322	5)	(333	8)	(334	4)	(335	5)	(337	3)
(338	6)	(339	3)	(343	3)	(344	4)	(345	3)
(346	3)	(347	4)	(348	10)	(353	3)	(354	3)
(359	8)	(361	8)	(365	4)	(367	3)	(376	3)
(377	5)	(378	4)	(389	4)	(390	6)	(392	5)
(395	5)	(411	4)	(420	6)	(421	4)	(424	5)
(425	3)	(428	3)	(435	3)	(448	13)	(449	47)
(450	26)	(451	18)	(466	6)	(467	3)	(469	4)
(470	5)	(473	3)	(475	4)	(478	4)	(484	3)
(488	5)	(493	3)	(495	5)	(498	7)	(500	5)
(507	3)	(512	4)	(514	5)	(515	6)	(525	3)
(529	5)	(530	3)	(533	6)	(534	8)	(543	6)
(547	5)	(553	4)	(557	4)	(567	3)	(575	3)
(595	4)								

NAME:12C_2023.2_1160EC43_[766; beta-D-Methylglucopyranoside (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203003-10-1

RI:2023

RT:13.133

NUM PEAKS: 92

(70	4)	(71	3)	(72	17)	(73	1000)	(74	84)
(75	90)	(76	5)	(77	5)	(81	5)	(83	4)
(84	7)	(85	4)	(86	3)	(87	4)	(88	3)
(89	75)	(90	7)	(91	7)	(97	4)	(99	5)
(100	46)	(101	23)	(102	17)	(103	75)	(104	8)
(105	10)	(111	3)	(113	6)	(115	9)	(116	12)
(117	34)	(118	4)	(119	7)	(127	3)	(128	4)
(129	68)	(130	13)	(131	26)	(132	12)	(133	48)
(134	6)	(135	4)	(142	5)	(143	15)	(144	3)
(145	6)	(147	176)	(148	57)	(149	25)	(150	3)
(155	4)	(157	32)	(158	6)	(159	4)	(160	7)
(161	5)	(163	7)	(169	9)	(170	3)	(172	8)
(173	3)	(174	3)	(175	3)	(177	3)	(189	36)
(190	10)	(191	22)	(192	4)	(203	8)	(204	398)
(205	97)	(206	38)	(207	8)	(217	85)	(218	23)
(219	10)	(220	80)	(221	18)	(222	7)	(229	5)
(230	5)	(231	6)	(233	13)	(234	3)	(243	9)
(244	4)	(259	6)	(291	3)	(305	4)	(319	69)
(320	23)	(321	11)						

NAME:12C_2002.2_1178EC16_[775; Dopamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200002-10-1

RI:2002

RT:12.973

NUM PEAKS: 186

(70	70)	(72	16)	(73	932)	(74	101)	(75	182)
(76	10)	(77	8)	(80	10)	(82	14)	(84	13)
(86	211)	(87	27)	(88	6)	(89	6)	(90	4)
(94	28)	(95	3)	(96	11)	(98	21)	(99	5)
(100	103)	(101	17)	(102	32)	(103	14)	(104	5)

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(105	5)	(106	4)	(110	4)	(111	7)	(112	23)
(113	6)	(114	19)	(115	15)	(116	42)	(117	19)
(118	7)	(119	5)	(121	5)	(122	3)	(123	3)
(126	5)	(128	29)	(129	9)	(130	74)	(131	41)
(132	16)	(133	30)	(134	7)	(135	7)	(138	3)
(139	9)	(140	7)	(141	3)	(142	107)	(143	21)
(144	17)	(146	31)	(147	77)	(148	16)	(149	20)
(150	7)	(151	4)	(152	9)	(153	3)	(154	8)
(156	11)	(158	13)	(159	5)	(160	4)	(161	5)
(163	4)	(166	4)	(168	9)	(169	4)	(170	24)
(171	14)	(172	28)	(173	18)	(174	1000)	(175	174)
(176	77)	(177	9)	(184	12)	(186	44)	(187	7)
(188	5)	(190	4)	(195	4)	(196	4)	(199	3)
(200	19)	(201	6)	(202	5)	(203	3)	(204	3)
(206	3)	(208	3)	(209	3)	(211	10)	(212	3)
(213	4)	(214	45)	(215	10)	(216	12)	(220	3)
(221	3)	(222	4)	(227	6)	(228	14)	(229	7)
(230	8)	(231	3)	(232	3)	(244	7)	(246	3)
(252	3)	(258	6)	(260	3)	(261	20)	(262	6)
(263	3)	(270	3)	(272	3)	(274	3)	(281	3)
(285	6)	(286	7)	(287	4)	(289	8)	(298	3)
(301	5)	(303	3)	(314	3)	(317	34)	(318	13)
(319	4)	(320	3)	(323	3)	(331	3)	(332	3)
(344	3)	(352	3)	(353	3)	(357	4)	(362	3)
(375	23)	(376	9)	(377	7)	(378	3)	(388	3)
(389	5)	(390	6)	(395	3)	(397	3)	(403	4)
(404	3)	(408	3)	(413	3)	(415	3)	(425	3)
(429	3)	(432	3)	(433	3)	(436	3)	(440	3)
(444	3)	(455	3)	(461	3)	(466	3)	(467	4)
(480	4)	(481	4)	(491	3)	(502	4)	(503	3)
(514	5)	(517	3)	(522	4)	(523	3)	(526	3)
(528	3)	(535	3)	(547	3)	(549	4)	(550	3)
(551	4)								

NAME:12C_1882.5_1274EC11_Mannose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188002-10-1

RI:1883

RT:12.225

NUM PEAKS: 114

(72	6)	(73	1000)	(74	78)	(75	158)	(76	43)
(77	12)	(81	6)	(85	3)	(87	3)	(88	5)
(89	36)	(90	3)	(91	9)	(93	19)	(94	4)
(97	5)	(99	10)	(100	10)	(101	28)	(102	11)
(103	139)	(104	47)	(105	32)	(106	7)	(111	3)
(113	5)	(115	11)	(116	17)	(117	114)	(118	13)
(119	16)	(120	3)	(121	16)	(122	7)	(123	6)
(126	6)	(127	5)	(129	183)	(130	32)	(131	43)
(132	15)	(134	3)	(135	8)	(138	5)	(141	3)
(142	8)	(143	24)	(144	5)	(145	10)	(147	118)
(148	19)	(151	7)	(154	4)	(155	4)	(156	3)
(157	138)	(158	23)	(159	11)	(163	26)	(164	4)
(167	20)	(168	4)	(169	13)	(170	4)	(171	7)
(173	42)	(174	26)	(175	7)	(177	5)	(182	3)
(186	9)	(187	4)	(189	87)	(190	18)	(196	3)
(197	3)	(201	4)	(203	8)	(205	126)	(206	21)
(207	11)	(214	5)	(215	6)	(217	100)	(218	18)
(219	23)	(220	48)	(221	14)	(222	6)	(223	28)
(224	4)	(229	24)	(230	9)	(231	7)	(243	16)
(244	12)	(245	8)	(246	4)	(247	20)	(248	6)

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(249 3) (257 3) (259 5) (271 4) (277 3)
 (302 4) (304 5) (305 4) (306 3) (319 53)
 (320 14) (321 6) (333 8) (334 3)

NAME:12C 1882.4_1160EC15_Adenine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:188005-10-1
 RI:1882

RT:12.217

NUM PEAKS: 37

(73 675) (79 56) (81 27) (84 169) (86 45)
 (91 126) (95 59) (99 74) (103 15) (109 161)
 (110 61) (115 31) (117 21) (119 79) (120 56)
 (122 30) (137 34) (164 22) (165 80) (167 56)
 (176 17) (192 219) (193 42) (227 138) (264 1000)
 (265 190) (266 43) (270 9) (278 128) (279 206)
 (359 9) (413 24) (431 24) (462 10) (484 19)
 (500 12) (582 25)

NAME:12C 1850.9_1274EC11_[912; Tetradecanoic acid (1TMS)]
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:185004-10-1

RI:1851

RT:11.982

NUM PEAKS: 82

(70 17) (71 20) (72 43) (73 681) (74 70)
 (75 933) (76 67) (77 47) (79 19) (81 57)
 (83 42) (85 16) (87 5) (89 21) (90 4)
 (91 7) (93 15) (95 52) (96 7) (97 34)
 (98 31) (99 19) (101 11) (105 29) (107 8)
 (109 16) (111 17) (112 8) (115 6) (116 62)
 (117 1000) (118 99) (119 40) (121 6) (123 4)
 (125 5) (129 412) (130 43) (131 178) (132 449)
 (133 86) (134 22) (135 5) (141 3) (143 37)
 (144 3) (145 203) (146 24) (147 8) (153 3)
 (154 7) (155 3) (159 26) (167 5) (171 18)
 (173 8) (185 23) (186 3) (187 16) (188 4)
 (199 7) (201 49) (202 8) (203 3) (204 3)
 (213 9) (215 10) (216 3) (227 6) (229 3)
 (241 16) (242 4) (243 7) (257 19) (284 3)
 (285 222) (286 55) (287 15) (299 9) (300 30)
 (301 8) (302 3)

NAME:12C 1822.5_1313EC75_Citric acid (4TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:182004-10-1

RI:1823

RT:11.258

NUM PEAKS: 87

(70 7) (71 5) (72 35) (73 1000) (74 85)
 (75 185) (76 12) (77 22) (79 3) (83 3)
 (85 3) (87 4) (88 3) (95 5) (97 7)
 (99 17) (101 6) (111 9) (115 18) (116 9)
 (117 15) (118 3) (119 5) (129 25) (130 3)
 (131 28) (132 4) (133 46) (134 7) (135 6)
 (139 5) (141 8) (142 3) (143 17) (145 3)
 (147 288) (148 46) (149 48) (150 6) (151 4)
 (157 6) (163 5) (169 5) (171 6) (183 39)
 (184 6) (185 11) (189 4) (190 4) (191 5)
 (201 3) (207 7) (211 46) (212 7) (213 8)

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(215	7)	(217	10)	(221	20)	(222	5)	(223	3)
(229	5)	(231	11)	(232	3)	(245	3)	(257	23)
(258	6)	(259	5)	(273	171)	(274	39)	(275	17)
(285	6)	(301	4)	(303	5)	(305	10)	(306	3)
(347	32)	(348	11)	(349	6)	(363	22)	(364	7)
(365	3)	(375	26)	(376	9)	(377	5)	(465	9)
(466	5)	(467	3)						

NAME:12C_1824.3_1191EC08_[570; Hypoxanthine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:182006-10-1

RI:1824

RT:11.718

NUM PEAKS: 163

(71	177)	(74	499)	(79	33)	(80	60)	(81	31)
(85	268)	(86	997)	(90	10)	(91	279)	(98	29)
(99	87)	(100	809)	(102	373)	(104	78)	(105	781)
(106	124)	(107	7)	(108	8)	(109	35)	(110	55)
(111	29)	(112	89)	(113	12)	(114	40)	(118	70)
(119	103)	(120	56)	(121	30)	(123	111)	(124	55)
(125	151)	(126	50)	(138	29)	(140	57)	(144	25)
(145	61)	(152	36)	(154	61)	(159	15)	(165	9)
(166	101)	(170	15)	(172	118)	(173	82)	(178	19)
(179	15)	(180	23)	(181	81)	(182	30)	(184	19)
(187	16)	(188	70)	(190	16)	(191	58)	(192	55)
(193	99)	(194	22)	(195	10)	(197	22)	(198	25)
(199	33)	(201	48)	(202	16)	(203	19)	(204	24)
(205	31)	(206	153)	(207	8)	(208	22)	(214	33)
(215	18)	(219	19)	(220	25)	(226	21)	(227	6)
(229	99)	(230	32)	(234	21)	(238	30)	(239	24)
(241	308)	(242	128)	(243	31)	(244	21)	(248	9)
(249	26)	(250	17)	(251	10)	(252	20)	(253	4)
(254	6)	(258	222)	(259	82)	(260	14)	(261	8)
(262	11)	(263	10)	(264	20)	(265	1000)	(266	253)
(267	101)	(270	31)	(277	9)	(279	32)	(280	326)
(281	86)	(282	17)	(288	12)	(289	10)	(303	5)
(304	10)	(315	8)	(316	16)	(317	4)	(326	4)
(329	22)	(330	19)	(331	25)	(332	25)	(337	5)
(341	10)	(343	11)	(351	15)	(356	3)	(357	9)
(378	4)	(388	3)	(403	7)	(405	12)	(406	19)
(407	7)	(421	10)	(422	18)	(423	26)	(424	3)
(431	6)	(435	4)	(439	4)	(445	8)	(446	6)
(450	6)	(451	4)	(458	8)	(462	11)	(469	7)
(471	3)	(476	4)	(501	7)	(524	5)	(529	4)
(530	6)	(537	4)	(538	6)	(543	4)	(561	6)
(564	3)	(568	8)	(569	7)	(571	6)	(575	4)
(581	4)	(582	3)	(595	3)				

NAME:12C_1771.1_1274EC11_[812; D-Xylofuranose (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177004-10-1

RI:1771

RT:11.367

NUM PEAKS: 78

(70	6)	(72	13)	(73	1000)	(74	81)	(75	94)
(76	4)	(77	5)	(79	3)	(81	10)	(83	6)
(84	6)	(85	3)	(87	4)	(89	5)	(95	4)
(97	4)	(99	7)	(103	12)	(109	4)	(111	5)
(113	5)	(115	4)	(116	4)	(117	30)	(118	3)
(119	6)	(127	4)	(128	3)	(129	28)	(130	3)

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(131	11)	(133	47)	(141	4)	(142	7)	(143	19)
(144	7)	(145	6)	(147	226)	(148	35)	(149	35)
(150	4)	(155	5)	(157	7)	(159	6)	(161	3)
(163	9)	(169	20)	(170	4)	(171	3)	(177	4)
(189	5)	(191	38)	(203	15)	(204	5)	(205	3)
(215	3)	(217	523)	(218	137)	(219	55)	(220	9)
(221	5)	(231	5)	(232	56)	(233	15)	(234	6)
(243	6)	(245	6)	(255	3)	(257	16)	(258	4)
(271	4)	(305	16)	(306	5)	(307	3)	(318	3)
(450	18)	(451	10)	(452	5)				

NAME:12C_1710.6_1274EC17 [817; Ribitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1711 |RI:1711

CASNO:171008-10-1

RI:1711

RT:10.896

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 148

(72	16)	(73	1000)	(74	86)	(75	260)	(76	15)
(77	32)	(81	6)	(83	29)	(88	7)	(89	11)
(95	16)	(97	26)	(101	105)	(102	14)	(103	209)
(104	22)	(105	11)	(109	13)	(110	8)	(114	6)
(116	41)	(117	114)	(118	12)	(119	15)	(121	11)
(122	8)	(129	164)	(130	27)	(133	88)	(134	10)
(136	6)	(137	8)	(138	25)	(139	35)	(140	13)
(143	14)	(144	6)	(145	11)	(147	428)	(148	69)
(149	84)	(150	14)	(156	4)	(157	35)	(163	21)
(164	9)	(169	34)	(170	7)	(171	5)	(175	7)
(177	6)	(185	11)	(186	8)	(187	36)	(188	11)
(189	35)	(190	11)	(191	29)	(192	7)	(193	14)
(203	25)	(205	78)	(206	17)	(213	14)	(215	4)
(217	257)	(218	59)	(219	28)	(220	13)	(221	29)
(222	11)	(228	8)	(229	7)	(243	27)	(245	5)
(246	4)	(256	6)	(257	7)	(260	6)	(263	8)
(275	8)	(276	5)	(277	11)	(281	4)	(284	5)
(291	5)	(294	3)	(297	6)	(298	7)	(303	17)
(304	5)	(305	5)	(307	35)	(308	12)	(313	10)
(316	7)	(317	9)	(318	4)	(319	32)	(320	13)
(321	9)	(322	3)	(324	4)	(325	4)	(332	5)
(333	4)	(334	7)	(335	6)	(336	4)	(338	4)
(339	3)	(340	5)	(341	8)	(342	7)	(344	6)
(353	6)	(360	6)	(365	4)	(366	7)	(367	8)
(375	5)	(377	4)	(378	4)	(380	4)	(387	5)
(404	4)	(420	6)	(426	4)	(432	4)	(438	6)
(442	4)	(443	4)	(447	6)	(453	4)	(461	3)
(463	6)	(469	8)	(474	4)	(477	7)	(489	4)
(492	5)	(511	5)	(520	3)	(538	3)	(539	5)
(544	3)	(547	4)	(566	3)				

NAME:12C_1682.1_1160EC15_Aspargine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168001-10-1

RI:1682

RT:10.676

NUM PEAKS: 96

(70	21)	(71	6)	(72	41)	(73	1000)	(74	132)
(75	279)	(76	21)	(77	24)	(78	3)	(79	6)
(84	10)	(85	6)	(86	15)	(87	7)	(88	4)
(89	9)	(90	8)	(91	3)	(98	13)	(99	7)
(100	120)	(101	15)	(102	15)	(103	48)	(104	5)

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(105	5)	(113	4)	(114	26)	(115	33)	(116	427)
(117	60)	(118	23)	(119	6)	(125	10)	(126	3)
(127	3)	(128	21)	(129	10)	(130	34)	(131	75)
(132	209)	(133	65)	(134	15)	(135	5)	(140	3)
(141	119)	(142	23)	(143	13)	(144	16)	(145	4)
(146	8)	(147	161)	(148	28)	(149	25)	(150	3)
(156	3)	(158	6)	(159	48)	(160	10)	(161	4)
(163	3)	(169	8)	(172	12)	(173	4)	(174	9)
(188	122)	(189	27)	(190	18)	(191	4)	(199	4)
(202	36)	(203	9)	(204	14)	(205	5)	(206	3)
(213	3)	(214	3)	(215	17)	(216	11)	(217	20)
(218	37)	(219	8)	(220	4)	(229	3)	(231	147)
(232	33)	(233	14)	(243	8)	(244	4)	(245	3)
(258	25)	(259	7)	(307	5)	(316	4)	(333	7)
(348	7)								

NAME:12C_1653.8_1191EC10_[548; Leucine (2TBS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:165002-10-1

RT:1654

RT:10.407

NUM PEAKS: 176

(72	23)	(73	1000)	(74	85)	(81	6)	(82	9)
(84	5)	(86	16)	(87	5)	(88	3)	(89	12)
(90	6)	(93	12)	(94	4)	(97	3)	(100	73)
(101	9)	(102	8)	(103	6)	(105	4)	(107	6)
(109	6)	(110	9)	(112	17)	(114	36)	(115	5)
(121	3)	(122	3)	(125	3)	(126	19)	(128	6)
(130	33)	(131	24)	(132	11)	(133	37)	(135	8)
(137	3)	(138	3)	(140	16)	(141	5)	(142	37)
(143	6)	(144	5)	(146	17)	(147	80)	(148	12)
(149	12)	(150	5)	(152	3)	(153	8)	(154	5)
(155	4)	(157	6)	(158	7)	(159	4)	(160	11)
(161	7)	(163	13)	(164	25)	(165	10)	(167	5)
(170	6)	(171	4)	(172	63)	(173	14)	(174	27)
(178	5)	(179	30)	(181	3)	(185	3)	(186	11)
(187	4)	(188	3)	(193	4)	(194	3)	(198	7)
(199	5)	(200	120)	(201	32)	(202	11)	(203	3)
(211	3)	(213	8)	(214	5)	(215	3)	(216	18)
(217	11)	(218	3)	(220	4)	(225	6)	(227	7)
(236	3)	(241	3)	(243	8)	(245	3)	(249	3)
(252	16)	(253	8)	(254	3)	(268	8)	(270	3)
(271	7)	(272	4)	(281	7)	(285	3)	(289	3)
(296	9)	(298	5)	(301	6)	(302	6)	(305	3)
(310	3)	(311	4)	(313	3)	(314	4)	(315	70)
(316	22)	(317	12)	(321	4)	(329	5)	(330	8)
(331	3)	(337	3)	(338	7)	(342	3)	(345	7)
(346	4)	(347	3)	(354	3)	(357	3)	(359	3)
(364	3)	(365	3)	(366	4)	(367	4)	(371	5)
(376	3)	(377	4)	(378	3)	(382	4)	(386	3)
(390	3)	(391	3)	(393	3)	(394	3)	(407	3)
(409	4)	(412	5)	(417	4)	(418	3)	(419	3)
(424	3)	(435	3)	(436	5)	(440	4)	(441	3)
(448	3)	(453	5)	(462	3)	(463	3)	(480	3)
(483	3)	(484	5)	(495	3)	(498	3)	(499	4)
(507	3)	(511	3)	(513	3)	(522	3)	(533	3)
(543	3)	(545	5)	(546	4)	(549	3)	(557	3)
(563	3)								

NAME:12C_1509.3_1178EC16_[622; Parabanic acid (2TMS)]

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:151002-10-1

RI:1509

RT:9.317

NUM PEAKS: 26

(79	86)	(100	1000)	(101	75)	(102	56)	(115	834)
(116	156)	(128	479)	(131	79)	(144	20)	(153	13)
(158	66)	(171	52)	(201	43)	(202	15)	(207	39)
(243	342)	(244	68)	(245	30)	(257	6)	(261	12)
(431	6)	(457	4)	(518	9)	(523	10)	(544	7)
(568	7)								

NAME:12C_1481.5_1160EC15_{815; (E)-4-Methyl-5-hydroxy-3-penten-2-one
(1TMS)}

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148002-10-1

RI:1482

RT:9.067

NUM PEAKS: 16

(72	9)	(73	424)	(74	52)	(76	48)	(82	21)
(84	43)	(100	70)	(112	5)	(139	175)	(147	54)
(148	11)	(155	1000)	(156	183)	(229	28)	(372	15)
(526	18)								

NAME:12C_1467.9_1178EC16_{709; 2,5-Diaminovalerolactam (2TMS)}

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147003-10-1

RI:1468

RT:8.883

NUM PEAKS: 105

(70	239)	(71	24)	(72	70)	(73	1000)	(74	128)
(75	164)	(76	13)	(77	11)	(80	13)	(82	16)
(83	8)	(84	33)	(85	20)	(86	85)	(87	21)
(88	12)	(89	11)	(95	12)	(96	10)	(97	11)
(98	35)	(99	20)	(100	413)	(101	52)	(102	47)
(103	14)	(104	3)	(105	5)	(106	5)	(110	11)
(111	5)	(112	22)	(113	32)	(114	45)	(115	449)
(116	64)	(117	31)	(118	6)	(119	4)	(124	4)
(125	4)	(126	38)	(127	21)	(128	682)	(129	87)
(130	52)	(131	70)	(132	21)	(133	35)	(134	6)
(135	3)	(137	12)	(138	3)	(139	4)	(140	15)
(141	292)	(142	91)	(143	23)	(144	20)	(145	3)
(146	12)	(147	200)	(148	33)	(149	16)	(152	6)
(153	56)	(154	35)	(155	18)	(156	15)	(157	5)
(158	16)	(159	4)	(160	4)	(167	5)	(168	11)
(169	145)	(170	26)	(171	22)	(172	11)	(173	3)
(174	71)	(175	13)	(176	5)	(185	4)	(186	5)
(187	4)	(188	8)	(200	4)	(203	20)	(204	4)
(214	3)	(215	12)	(216	26)	(217	6)	(227	4)
(229	8)	(230	3)	(241	6)	(242	3)	(243	199)
(244	43)	(245	17)	(257	4)	(258	20)	(259	5)

NAME:12C_1474.4_1191EC10_{NA}

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:147002-10-1

RI:1474

RT:8.933

NUM PEAKS: 136

(70	1000)	(71	77)	(72	122)	(74	33)	(75	427)
(76	48)	(77	13)	(78	14)	(79	3)	(82	5)

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( 84 123) ( 86 74) ( 87 13) ( 88 11) ( 89 3)
( 90 51) ( 91 6) ( 92 4) ( 94 4) ( 95 3)
( 97 18) ( 98 68) (100 79) (101 40) (102 14)
(103 11) (104 7) (105 6) (106 4) (107 3)
(111 5) (114 17) (115 31) (116 14) (117 27)
(118 6) (119 4) (122 3) (129 9) (130 28)
(131 27) (132 25) (133 61) (134 14) (135 10)
(136 3) (140 4) (142 100) (143 24) (144 11)
(146 7) (147 14) (148 17) (149 17) (150 6)
(151 4) (153 3) (157 7) (158 12) (159 34)
(160 16) (161 4) (163 3) (164 3) (167 4)
(168 3) (169 3) (170 5) (171 21) (172 8)
(173 5) (174 23) (175 8) (176 6) (184 3)
(185 9) (186 7) (188 7) (190 5) (197 3)
(200 3) (203 4) (204 6) (211 6) (212 3)
(213 3) (216 4) (217 7) (218 65) (219 16)
(220 8) (230 4) (236 7) (240 3) (241 7)
(242 3) (248 8) (256 6) (259 7) (260 5)
(261 4) (273 3) (275 3) (276 12) (277 5)
(292 10) (293 7) (294 4) (305 3) (307 3)
(319 3) (320 15) (321 6) (322 4) (336 3)
(353 4) (354 4) (362 3) (372 3) (376 3)
(407 3) (408 3) (421 3) (422 3) (428 3)
(429 3) (430 3) (435 3) (436 3) (444 3)
(464 3) (465 3) (478 3) (483 3) (490 3)
(494 3)

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NAME:12C 1296.5 1191EC10_Phosporic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129001-10-1

RI:1297

RT:6.913

NUM PEAKS: 89

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( 70 7) ( 71 11) ( 72 26) ( 73 1000) ( 74 106)
( 75 97) ( 76 5) ( 77 37) ( 79 6) ( 84 3)
( 85 7) ( 87 12) ( 88 4) ( 89 19) ( 91 10)
(102 5) (103 83) (104 13) (105 28) (106 4)
(107 15) (109 5) (113 3) (115 53) (116 11)
(119 39) (120 6) (121 22) (122 3) (123 10)
(131 36) (132 8) (133 250) (134 34) (135 68)
(136 8) (137 35) (138 4) (139 3) (145 4)
(150 4) (151 23) (152 3) (153 5) (163 8)
(165 13) (166 4) (167 13) (176 3) (177 11)
(178 4) (179 9) (180 3) (181 36) (182 6)
(183 13) (184 3) (189 13) (190 4) (191 50)
(192 12) (193 53) (194 10) (195 14) (196 3)
(197 4) (207 54) (208 11) (209 9) (210 3)
(211 128) (212 19) (213 10) (221 5) (225 24)
(226 5) (227 7) (269 4) (283 24) (284 9)
(285 4) (298 8) (299 436) (300 112) (301 58)
(302 10) (314 62) (315 16) (316 8)

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NAME:12C 1220.2 1274EC17_Valine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:122001-10-1

RI:1220

RT:6.122

NUM PEAKS: 55

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( 70 15) ( 71 6) ( 72 60) ( 73 846) ( 74 82)
( 75 98) ( 76 7) ( 77 4) ( 82 6) ( 83 4)

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(84	4)	(85	5)	(86	13)	(87	5)	(98	4)
(99	4)	(100	114)	(101	16)	(102	9)	(103	24)
(104	3)	(105	3)	(112	4)	(114	9)	(115	7)
(116	3)	(117	11)	(118	3)	(119	3)	(128	19)
(129	12)	(130	12)	(131	15)	(132	17)	(133	26)
(134	4)	(142	6)	(143	5)	(144	1000)	(145	134)
(146	49)	(147	153)	(148	24)	(149	14)	(156	22)
(157	4)	(158	3)	(160	3)	(163	4)	(174	4)
(203	3)	(218	143)	(219	34)	(220	13)	(246	9)

NAME:12C_1282.1_1274EC17_Serine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:128001-10-1
 RI:1282

RT:6.820

NUM PEAKS: 62

(70	19)	(71	6)	(72	25)	(73	961)	(74	123)
(75	316)	(76	31)	(81	15)	(84	3)	(85	6)
(86	71)	(87	24)	(88	36)	(89	16)	(90	6)
(91	10)	(96	4)	(98	4)	(99	5)	(100	110)
(101	24)	(102	29)	(103	134)	(104	14)	(105	7)
(114	8)	(115	9)	(116	1000)	(117	112)	(118	43)
(119	6)	(128	3)	(130	71)	(131	37)	(132	761)
(133	118)	(134	35)	(142	3)	(143	4)	(144	134)
(145	16)	(146	76)	(147	99)	(148	19)	(149	15)
(159	57)	(160	8)	(161	4)	(172	3)	(188	17)
(189	5)	(190	4)	(206	5)	(216	5)	(217	4)
(219	33)	(220	7)	(221	3)	(234	31)	(235	7)
(236	3)	(262	3)						

NAME:12C_1326.5_1274EC17_Glycine (3TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:133001-10-1

RI:1327

RT:7.320

NUM PEAKS: 48

(71	4)	(72	14)	(73	561)	(74	44)	(85	4)
(86	340)	(87	29)	(88	13)	(99	3)	(100	189)
(101	30)	(102	23)	(103	10)	(105	3)	(113	5)
(115	4)	(116	7)	(119	8)	(131	21)	(133	99)
(134	14)	(135	7)	(144	6)	(147	290)	(148	46)
(149	23)	(158	7)	(159	3)	(160	21)	(161	4)
(172	10)	(173	3)	(174	1000)	(175	189)	(176	83)
(177	18)	(188	8)	(202	3)	(204	4)	(246	11)
(247	4)	(248	139)	(249	42)	(250	19)	(251	3)
(276	52)	(277	14)	(278	7)				

NAME:12C_1352.5_1274EC17_Glyceric acid (3TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:135003-10-1

RI:1353

RT:7.614

NUM PEAKS: 78

(70	47)	(71	197)	(72	20)	(73	1000)	(74	74)
(82	11)	(83	10)	(84	28)	(85	99)	(89	9)
(97	3)	(99	22)	(101	28)	(102	169)	(103	170)
(104	20)	(105	8)	(106	4)	(109	5)	(111	6)
(113	21)	(115	12)	(116	11)	(117	88)	(118	6)
(119	11)	(124	4)	(125	3)	(126	10)	(127	16)
(130	66)	(131	35)	(133	169)	(141	3)	(145	4)

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(147	458)	(148	54)	(149	23)	(152	3)	(155	7)
(162	4)	(163	7)	(168	5)	(169	13)	(173	4)
(175	9)	(177	8)	(179	3)	(188	3)	(189	311)
(190	50)	(191	27)	(196	7)	(204	10)	(205	64)
(206	9)	(207	7)	(212	6)	(216	4)	(217	16)
(221	30)	(222	10)	(226	14)	(236	4)	(241	4)
(249	3)	(251	3)	(256	7)	(267	18)	(268	8)
(278	4)	(281	10)	(292	100)	(293	31)	(294	10)
(297	3)	(306	3)	(307	25)				

NAME:12C_1394.9_1274EC17_[644; 2-Methyl-1,3-butanediol (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140003-10-1

RI:1395

RT:8.092

NUM PEAKS: 50

(71	81)	(72	29)	(73	1000)	(74	85)	(75	259)
(76	23)	(101	43)	(102	7)	(115	29)	(116	193)
(117	836)	(118	85)	(119	39)	(129	20)	(130	5)
(131	33)	(133	123)	(134	25)	(143	175)	(144	47)
(145	33)	(147	405)	(148	67)	(149	140)	(150	15)
(163	9)	(175	16)	(176	6)	(189	5)	(203	31)
(204	7)	(217	21)	(221	15)	(233	62)	(234	98)
(235	25)	(236	8)	(245	30)	(246	9)	(291	6)
(293	4)	(299	5)	(305	6)	(306	107)	(307	36)
(308	18)	(309	5)	(335	11)	(389	4)	(405	5)

NAME:12C_1403.1_1274EC17_Threonine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:140001-10-1

RI:1403

RT:8.183

NUM PEAKS: 98

(71	5)	(72	23)	(73	1000)	(74	93)	(75	109)
(76	8)	(84	10)	(85	7)	(86	19)	(87	19)
(88	6)	(89	15)	(98	5)	(99	5)	(100	93)
(101	187)	(102	29)	(104	4)	(105	8)	(106	2)
(112	4)	(113	3)	(114	22)	(115	22)	(116	9)
(117	303)	(118	34)	(119	27)	(120	3)	(128	70)
(129	88)	(130	53)	(131	50)	(132	46)	(133	71)
(134	17)	(135	22)	(142	3)	(144	6)	(145	4)
(146	13)	(147	176)	(148	31)	(149	21)	(150	4)
(156	3)	(158	7)	(159	9)	(160	9)	(161	3)
(163	8)	(165	3)	(172	6)	(174	6)	(175	3)
(176	4)	(177	7)	(178	3)	(186	5)	(188	4)
(189	5)	(190	4)	(191	18)	(192	13)	(193	14)
(202	25)	(203	28)	(204	12)	(206	5)	(207	23)
(208	12)	(209	5)	(212	2)	(216	4)	(217	3)
(218	211)	(219	239)	(220	57)	(224	20)	(226	4)
(230	7)	(231	3)	(240	8)	(244	2)	(248	2)
(269	4)	(282	14)	(283	6)	(284	3)	(291	56)
(292	35)	(293	14)	(294	5)	(316	2)	(320	10)
(321	5)	(329	5)	(344	5)				

NAME:12C_1414.0_1274EC17_[590; 1-Acetyl-2-thiohydantoin]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:141004-10-1

RI:1414

RT:8.306

NUM PEAKS: 71

163

(70 11) (72 79) (73 774) (74 215) (75 1000)
 (76 99) (77 76) (78 6) (79 12) (80 3)
 (82 9) (83 53) (84 39) (85 11) (86 28)
 (87 37) (88 13) (89 17) (90 4) (91 19)
 (92 3) (93 14) (95 5) (98 40) (99 10)
 (100 29) (101 107) (102 29) (103 72) (104 8)
 (105 30) (106 3) (112 16) (113 10) (114 117)
 (115 20) (116 756) (117 246) (118 30) (119 11)
 (126 4) (128 17) (129 50) (130 521) (131 67)
 (132 24) (140 24) (141 4) (142 8) (143 10)
 (144 23) (145 7) (146 104) (148 73) (149 9)
 (150 3) (156 29) (157 12) (158 278) (159 35)
 (160 14) (172 7) (173 37) (174 9) (176 22)
 (190 7) (191 3) (200 13) (215 4) (218 6)
 (233 3)

NAME:12C_1440.3_1274EC17_[678; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:144003-10-1

RI:1440

RT:8.603

NUM PEAKS: 63

(70 58) (71 6) (72 32) (73 1000) (74 117)
 (75 312) (76 30) (77 16) (84 4) (85 4)
 (86 10) (87 8) (88 6) (89 8) (91 5)
 (98 6) (99 7) (100 53) (101 11) (102 21)
 (103 13) (115 7) (116 223) (117 264) (118 36)
 (119 12) (128 17) (129 7) (130 310) (131 48)
 (132 20) (133 24) (134 4) (135 3) (143 3)
 (144 43) (145 6) (146 27) (147 133) (148 24)
 (149 18) (150 3) (159 25) (160 581) (161 73)
 (162 26) (172 10) (174 6) (187 7) (190 3)
 (202 21) (203 4) (220 16) (221 3) (234 33)
 (235 8) (236 3) (244 7) (245 50) (246 11)
 (247 4) (262 17) (263 3)

NAME:12C_1488.2_1274EC17_Malic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149001-10-1

RI:1488

RT:9.143

NUM PEAKS: 79

(70 7) (72 30) (73 1000) (74 84) (75 146)
 (76 13) (77 12) (78 3) (82 5) (83 3)
 (84 47) (87 6) (93 5) (99 6) (101 77)
 (102 8) (103 13) (105 5) (111 3) (115 10)
 (116 12) (117 53) (118 6) (119 9) (129 10)
 (131 35) (132 6) (133 126) (134 17) (135 12)
 (143 21) (144 5) (145 5) (146 3) (147 505)
 (148 76) (149 48) (150 4) (151 6) (171 24)
 (172 4) (173 4) (175 48) (176 8) (177 13)
 (185 3) (189 63) (190 48) (191 40) (192 9)
 (193 3) (203 5) (205 3) (217 25) (218 6)
 (219 3) (221 12) (222 3) (233 112) (234 22)
 (235 8) (245 66) (246 12) (247 8) (260 3)
 (263 14) (264 4) (265 20) (266 4) (305 4)
 (306 7) (307 21) (308 9) (309 4) (319 5)
 (320 3) (335 26) (336 6) (337 4)

NAME:12C_1565.1_1274EC17_Phenylalanine (1TMS)

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COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157001-10-1

RI:1565

RT:9.777

NUM PEAKS: 49

(72	4)	(73	277)	(74	82)	(75	218)	(76	24)
(77	75)	(78	12)	(79	3)	(80	3)	(86	17)
(87	14)	(88	4)	(89	14)	(90	8)	(91	163)
(92	29)	(93	28)	(94	3)	(100	6)	(102	15)
(103	105)	(104	17)	(105	4)	(116	3)	(117	10)
(118	42)	(119	26)	(120	1000)	(121	96)	(122	3)
(130	233)	(131	38)	(132	9)	(146	460)	(147	48)
(148	19)	(149	3)	(160	3)	(161	3)	(176	11)
(177	14)	(178	3)	(194	10)	(204	37)	(205	11)
(206	3)	(222	30)	(223	5)	(237	3)		

NAME:12C_1573.9_1274EC17_[708; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:157002-10-1

RI:1574

RT:9.844

NUM PEAKS: 85

(70	9)	(71	25)	(72	20)	(73	1000)	(74	85)
(75	205)	(76	13)	(77	7)	(81	5)	(83	21)
(85	16)	(87	3)	(89	9)	(95	9)	(97	45)
(98	7)	(99	17)	(101	7)	(102	3)	(103	14)
(110	3)	(111	6)	(113	9)	(115	5)	(117	49)
(119	4)	(127	5)	(131	22)	(132	3)	(133	81)
(134	12)	(135	9)	(141	5)	(143	141)	(144	17)
(145	9)	(147	442)	(148	69)	(149	88)	(150	10)
(151	4)	(157	71)	(158	11)	(161	8)	(169	5)
(171	9)	(177	11)	(184	3)	(185	5)	(189	3)
(190	5)	(191	156)	(192	27)	(193	12)	(213	16)
(217	21)	(218	3)	(220	5)	(221	15)	(222	3)
(231	47)	(232	11)	(233	7)	(243	18)	(244	3)
(245	5)	(259	4)	(265	38)	(266	10)	(267	3)
(275	128)	(276	30)	(277	11)	(287	15)	(288	3)
(289	3)	(299	3)	(305	16)	(306	6)	(307	3)
(349	5)	(350	3)	(377	20)	(378	8)	(379	3)

NAME:12C_1581.5_1274EC17_[680; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158003-10-1

RI:1582

RT:9.903

NUM PEAKS: 109

(70	11)	(71	120)	(72	29)	(73	1000)	(74	88)
(75	251)	(76	17)	(77	11)	(81	5)	(83	4)
(85	8)	(87	6)	(89	4)	(91	37)	(92	4)
(93	3)	(95	21)	(96	4)	(97	24)	(99	11)
(101	7)	(102	3)	(103	12)	(105	4)	(113	61)
(114	5)	(115	66)	(116	10)	(117	70)	(118	7)
(119	9)	(123	11)	(127	5)	(129	38)	(130	5)
(131	40)	(132	7)	(133	80)	(134	11)	(135	9)
(141	14)	(142	3)	(143	43)	(144	7)	(145	6)
(147	493)	(148	78)	(149	95)	(150	13)	(151	6)
(157	108)	(158	18)	(159	8)	(161	3)	(163	20)
(164	3)	(169	18)	(170	3)	(171	10)	(173	4)
(175	4)	(177	3)	(185	50)	(186	9)	(187	5)
(189	12)	(190	6)	(191	10)	(197	4)	(203	5)

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(204	5)	(205	4)	(207	4)	(212	4)	(213	49)
(214	8)	(215	5)	(217	37)	(218	8)	(219	6)
(221	20)	(222	5)	(223	3)	(231	62)	(232	19)
(233	10)	(243	6)	(245	6)	(259	62)	(260	16)
(261	28)	(262	6)	(275	233)	(276	57)	(277	26)
(278	4)	(287	47)	(288	11)	(289	6)	(305	11)
(306	4)	(307	4)	(333	3)	(349	36)	(350	16)
(351	8)	(377	37)	(378	13)	(379	6)		

NAME:12C_1595.8_1274EC17_[639; Proline (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:159001-10-1

RI:1596

RT:10.013

NUM PEAKS: 51

(70	29)	(72	85)	(73	1000)	(74	92)	(75	92)
(78	5)	(86	12)	(87	5)	(89	3)	(96	6)
(98	8)	(99	26)	(100	19)	(101	9)	(102	6)
(105	8)	(106	3)	(107	4)	(113	6)	(115	6)
(116	5)	(119	3)	(126	7)	(129	6)	(131	19)
(132	3)	(133	37)	(134	4)	(140	8)	(142	829)
(143	112)	(144	32)	(147	203)	(148	30)	(149	13)
(170	15)	(171	4)	(172	6)	(186	681)	(187	95)
(188	27)	(193	4)	(216	126)	(217	34)	(218	11)
(244	9)	(288	65)	(289	15)	(290	6)	(303	10)
(304	3)								

NAME:12C_1625.9_1274EC17_Glutamic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:163001-10-1

RI:1626

RT:10.245

NUM PEAKS: 104

(70	9)	(71	5)	(72	36)	(73	1000)	(74	108)
(75	342)	(76	18)	(77	8)	(82	7)	(83	9)
(84	343)	(85	26)	(86	12)	(87	8)	(88	3)
(89	5)	(95	6)	(96	3)	(98	10)	(99	4)
(100	97)	(101	19)	(102	10)	(103	11)	(112	13)
(113	11)	(114	22)	(115	21)	(116	4)	(117	23)
(118	3)	(119	7)	(126	3)	(128	392)	(129	67)
(130	31)	(131	31)	(132	23)	(133	68)	(134	10)
(140	45)	(141	7)	(142	6)	(143	6)	(144	6)
(145	5)	(146	7)	(147	263)	(148	44)	(151	3)
(154	4)	(155	4)	(156	255)	(157	45)	(158	61)
(159	3)	(160	5)	(163	4)	(172	5)	(173	6)
(174	57)	(175	7)	(186	11)	(188	4)	(189	5)
(191	3)	(198	3)	(201	3)	(202	8)	(203	6)
(204	33)	(205	7)	(206	4)	(214	10)	(215	4)
(216	6)	(218	35)	(219	10)	(220	4)	(221	12)
(229	3)	(230	117)	(231	28)	(232	13)	(245	11)
(246	695)	(247	149)	(248	63)	(249	8)	(258	19)
(259	5)	(260	3)	(273	3)	(274	6)	(276	5)
(299	4)	(320	6)	(321	3)	(348	32)	(349	10)
(350	5)	(363	15)	(364	6)	(365	3)		

NAME:12C_1770.3_1274EC17_[NA]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:177003-10-1

RI:1770

RT:11.356

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NUM PEAKS: 52

(82	47)	(84	40)	(86	615)	(100	394)	(112	34)
(125	11)	(126	8)	(128	12)	(140	40)	(141	4)
(144	60)	(156	194)	(157	32)	(158	136)	(160	21)
(169	5)	(170	4)	(171	5)	(172	796)	(173	278)
(174	1000)	(175	157)	(176	61)	(185	40)	(187	27)
(199	262)	(200	86)	(201	27)	(202	12)	(214	38)
(215	10)	(217	14)	(230	9)	(231	5)	(239	41)
(244	157)	(245	27)	(246	50)	(247	3)	(273	21)
(274	6)	(305	4)	(329	87)	(330	206)	(331	89)
(332	34)	(345	165)	(346	64)	(347	22)	(361	16)
(362	13)	(363	5)						

NAME:12C_1794.4_1274EC17_[789; Tyramine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179002-10-1

RI:1794

RT:11.541

NUM PEAKS: 53

(72	9)	(73	612)	(74	57)	(75	158)	(76	8)
(86	350)	(87	23)	(88	4)	(89	93)	(90	4)
(100	127)	(101	19)	(102	38)	(105	4)	(117	19)
(118	5)	(128	6)	(129	39)	(130	48)	(131	9)
(144	6)	(146	27)	(147	4)	(148	6)	(156	12)
(160	29)	(161	4)	(167	7)	(174	1000)	(175	185)
(176	78)	(183	6)	(190	70)	(191	7)	(199	10)
(217	3)	(223	14)	(230	3)	(231	7)	(238	4)
(239	3)	(244	3)	(246	7)	(255	5)	(260	3)
(287	4)	(331	4)	(345	80)	(346	30)	(347	10)
(348	3)	(361	16)	(362	6)				

NAME:12C_1806.4_1274EC17_[944; D-Mannopyranose (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181005-10-1

RI:1806

RT:11.634

NUM PEAKS: 148

(70	12)	(72	7)	(73	1000)	(74	88)	(75	73)
(81	23)	(83	24)	(87	9)	(89	28)	(93	10)
(94	5)	(95	4)	(96	7)	(97	26)	(98	5)
(103	56)	(105	10)	(106	8)	(108	4)	(109	5)
(110	3)	(111	15)	(112	3)	(116	3)	(117	81)
(118	6)	(120	4)	(123	4)	(125	13)	(129	109)
(130	20)	(131	35)	(132	5)	(133	56)	(134	8)
(137	4)	(143	23)	(145	7)	(147	201)	(148	42)
(149	27)	(150	5)	(152	6)	(153	3)	(157	17)
(161	5)	(165	4)	(166	4)	(169	7)	(170	3)
(171	5)	(175	10)	(187	3)	(189	56)	(190	19)
(191	567)	(192	97)	(193	40)	(194	15)	(203	22)
(204	839)	(205	159)	(206	66)	(207	14)	(209	5)
(210	5)	(217	141)	(218	37)	(219	16)	(220	6)
(221	8)	(222	8)	(223	6)	(230	5)	(231	22)
(232	5)	(233	6)	(234	4)	(237	18)	(238	7)
(243	13)	(244	3)	(245	4)	(250	4)	(252	3)
(253	3)	(258	3)	(259	4)	(264	3)	(265	8)
(271	6)	(272	3)	(279	7)	(284	3)	(290	3)
(291	10)	(292	6)	(298	3)	(305	15)	(306	8)
(307	4)	(312	13)	(317	8)	(319	3)	(323	5)
(325	4)	(327	3)	(333	3)	(345	13)	(346	3)
(367	5)	(368	8)	(369	4)	(370	5)	(384	3)

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(393	7)	(394	5)	(397	4)	(398	3)	(403	4)
(404	4)	(413	4)	(423	6)	(426	4)	(434	6)
(435	10)	(437	4)	(438	5)	(439	3)	(458	6)
(463	5)	(473	4)	(474	4)	(475	4)	(479	3)
(485	8)	(489	3)	(490	4)	(493	4)	(498	5)
(519	3)	(526	5)	(527	5)	(541	3)	(549	5)
(553	4)	(560	4)	(570	4)				

NAME:12C_1868.5_1274EC17_[826; beta-[[5-methyl-2-thienyl)methylene]amino]-benzeneacetic acid methyl ester]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:187004-10-1

RI:1869

RT:12.112

NUM PEAKS: 78

(70	8)	(71	7)	(72	14)	(73	962)	(74	77)
(75	59)	(80	3)	(81	9)	(85	5)	(93	4)
(95	6)	(97	3)	(98	11)	(99	5)	(101	12)
(115	3)	(116	7)	(118	3)	(119	6)	(124	4)
(125	4)	(126	3)	(131	16)	(133	46)	(135	5)
(138	4)	(139	3)	(140	3)	(141	3)	(147	102)
(148	19)	(149	11)	(151	8)	(153	72)	(154	18)
(155	6)	(165	4)	(166	5)	(167	51)	(168	9)
(169	110)	(170	71)	(171	13)	(179	4)	(181	3)
(183	6)	(184	3)	(195	8)	(197	4)	(198	3)
(204	15)	(210	5)	(211	10)	(212	10)	(213	3)
(225	4)	(226	11)	(227	6)	(239	20)	(240	9)
(241	1000)	(242	248)	(243	96)	(244	13)	(267	13)
(268	4)	(269	4)	(284	4)	(315	6)	(341	3)
(343	3)	(356	6)	(374	3)	(431	18)	(432	9)
(433	4)	(446	5)	(447	3)				

NAME:12C_1877.4_1274EC17_alpha-D-Methylglucopyranoside (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:188006-10-1

RI:1877

RT:12.180

NUM PEAKS: 207

(70	203)	(73	1000)	(74	100)	(81	19)	(85	13)
(87	16)	(89	35)	(90	6)	(98	7)	(100	16)
(101	40)	(107	5)	(109	8)	(113	9)	(116	23)
(117	30)	(118	6)	(119	7)	(124	4)	(125	4)
(131	41)	(133	338)	(134	37)	(135	9)	(136	4)
(143	14)	(144	4)	(146	41)	(152	3)	(155	10)
(159	19)	(163	12)	(164	4)	(166	4)	(177	5)
(183	10)	(184	3)	(185	6)	(189	14)	(190	12)
(191	35)	(192	5)	(193	6)	(197	5)	(203	24)
(204	500)	(206	34)	(207	6)	(208	6)	(209	4)
(213	7)	(215	5)	(217	66)	(218	23)	(219	10)
(222	5)	(227	4)	(228	4)	(231	15)	(233	12)
(234	6)	(236	2)	(237	2)	(239	3)	(243	8)
(244	5)	(245	4)	(247	6)	(250	4)	(251	4)
(253	2)	(255	3)	(256	4)	(261	4)	(265	7)
(266	5)	(270	3)	(271	7)	(272	5)	(273	3)
(274	3)	(280	3)	(286	7)	(287	9)	(288	6)
(289	5)	(290	18)	(291	14)	(293	4)	(295	3)
(296	6)	(297	4)	(298	7)	(299	20)	(303	9)
(305	10)	(306	10)	(313	6)	(314	5)	(315	6)
(317	12)	(318	4)	(324	4)	(325	6)	(327	3)
(332	5)	(333	6)	(334	3)	(335	5)	(336	3)

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(337	6)	(338	3)	(341	4)	(345	4)	(349	4)
(353	4)	(361	7)	(371	3)	(372	2)	(374	3)
(376	3)	(377	6)	(381	3)	(382	3)	(385	2)
(386	7)	(387	4)	(388	5)	(391	5)	(393	4)
(396	4)	(399	4)	(400	3)	(405	3)	(408	3)
(409	4)	(412	3)	(413	3)	(414	6)	(415	5)
(429	3)	(430	4)	(431	3)	(436	4)	(437	9)
(438	8)	(439	4)	(446	4)	(448	4)	(450	2)
(451	5)	(454	3)	(456	3)	(457	4)	(461	2)
(464	5)	(469	6)	(472	4)	(473	5)	(476	4)
(477	3)	(478	3)	(480	4)	(482	6)	(485	3)
(486	5)	(489	5)	(490	5)	(491	4)	(495	5)
(496	5)	(497	4)	(501	7)	(503	6)	(507	5)
(508	3)	(510	4)	(511	6)	(514	6)	(515	5)
(517	5)	(518	3)	(521	6)	(524	4)	(526	3)
(529	7)	(533	4)	(535	3)	(536	3)	(538	4)
(539	5)	(541	4)	(547	6)	(548	3)	(549	3)
(553	3)	(557	4)	(559	3)	(563	4)	(565	2)
(567	2)	(568	2)	(569	2)	(574	2)	(576	2)
(578	2)	(584	2)						

NAME:12C 1889.9 1274EC17_Glucose methoxyamine (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:189002-10-1

RI:1890

RT:12.276

NUM PEAKS: 137

(70	5)	(71	6)	(72	20)	(73	1000)	(83	24)
(86	6)	(89	55)	(98	3)	(99	6)	(100	19)
(101	20)	(102	9)	(103	143)	(104	7)	(105	24)
(110	4)	(111	3)	(112	3)	(113	6)	(114	16)
(115	6)	(117	112)	(126	2)	(127	5)	(128	7)
(129	168)	(131	30)	(133	96)	(134	10)	(140	2)
(141	3)	(142	9)	(143	20)	(144	3)	(145	6)
(147	426)	(148	69)	(154	2)	(155	2)	(156	2)
(157	150)	(158	27)	(159	10)	(160	222)	(161	41)
(162	9)	(168	3)	(169	3)	(170	2)	(171	1)
(172	6)	(173	7)	(174	12)	(184	1)	(185	2)
(186	6)	(187	3)	(188	2)	(189	43)	(190	11)
(196	1)	(198	2)	(200	5)	(201	12)	(202	4)
(203	6)	(205	274)	(206	54)	(207	22)	(214	2)
(215	4)	(216	12)	(217	141)	(218	22)	(221	5)
(222	2)	(228	2)	(229	39)	(230	14)	(231	16)
(232	8)	(233	11)	(234	6)	(235	2)	(240	3)
(241	1)	(242	2)	(243	3)	(244	6)	(245	3)
(246	6)	(247	3)	(248	2)	(254	1)	(255	1)
(256	3)	(257	2)	(259	2)	(260	2)	(261	2)
(262	7)	(263	2)	(268	2)	(269	3)	(270	3)
(271	1)	(272	1)	(274	7)	(275	3)	(276	2)
(277	7)	(278	3)	(279	1)	(291	12)	(300	4)
(302	1)	(305	9)	(306	4)	(307	7)	(318	7)
(319	253)	(320	81)	(321	38)	(322	8)	(323	2)
(330	1)	(332	1)	(333	1)	(343	2)	(344	2)
(364	4)	(365	3)	(366	1)	(374	3)	(375	1)
(376	2)	(464	1)						

NAME:12C 1909.6 1274EC17_Glucose methoxyamine (BP) (5TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:191001-10-1

RI:1910

169

RT:12.415

NUM PEAKS: 65

(72	6)	(73	1000)	(74	77)	(75	66)	(76	3)
(89	62)	(90	3)	(91	3)	(101	11)	(103	186)
(104	17)	(105	23)	(116	4)	(117	84)	(118	7)
(119	8)	(129	127)	(130	8)	(131	23)	(133	83)
(134	10)	(135	6)	(143	12)	(145	3)	(147	304)
(148	42)	(149	28)	(150	3)	(157	97)	(158	11)
(159	8)	(160	134)	(161	27)	(162	7)	(163	12)
(177	6)	(189	30)	(190	24)	(191	15)	(201	6)
(203	3)	(204	24)	(205	195)	(206	41)	(207	21)
(214	3)	(217	86)	(218	16)	(219	6)	(221	6)
(229	27)	(233	16)	(234	4)	(235	6)	(243	3)
(277	9)	(278	5)	(291	7)	(300	3)	(305	4)
(307	5)	(319	183)	(320	57)	(321	26)	(322	5)

NAME:12C_1915.4_1274EC17_Lysine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192003-10-1

RI:1915

RT:12.451

NUM PEAKS: 122

(70	11)	(71	10)	(72	19)	(73	1000)	(74	110)
(75	73)	(76	5)	(77	3)	(82	20)	(83	5)
(84	36)	(85	15)	(86	123)	(87	16)	(88	57)
(89	6)	(90	4)	(94	5)	(97	3)	(98	11)
(99	10)	(100	115)	(101	17)	(102	37)	(103	13)
(104	3)	(110	4)	(112	32)	(113	10)	(114	34)
(115	36)	(116	16)	(117	22)	(118	5)	(119	5)
(124	3)	(126	15)	(127	4)	(128	157)	(129	24)
(130	51)	(131	32)	(132	23)	(133	31)	(134	6)
(135	3)	(138	3)	(139	3)	(140	31)	(141	8)
(142	21)	(143	5)	(144	7)	(145	3)	(146	30)
(147	98)	(148	20)	(149	10)	(150	3)	(151	10)
(152	3)	(154	36)	(155	19)	(156	540)	(157	80)
(158	34)	(159	5)	(160	11)	(161	3)	(162	3)
(166	7)	(167	4)	(168	7)	(170	5)	(172	20)
(173	5)	(174	501)	(175	94)	(176	43)	(177	5)
(179	11)	(184	5)	(186	14)	(187	4)	(188	6)
(189	4)	(191	11)	(200	55)	(201	12)	(202	17)
(203	4)	(204	3)	(212	4)	(213	4)	(214	15)
(215	7)	(216	8)	(218	19)	(219	8)	(220	5)
(228	31)	(229	9)	(230	118)	(231	26)	(232	12)
(240	3)	(244	3)	(255	3)	(258	6)	(272	6)
(273	8)	(274	4)	(317	110)	(318	39)	(319	15)
(320	3)	(329	11)	(330	5)	(419	3)	(434	12)
(435	7)	(436	3)						

NAME:12C_1938.9_1274EC17_Tyrosine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:194002-10-1

RI:1939

RT:12.600

NUM PEAKS: 79

(70	4)	(72	18)	(73	1000)	(74	94)	(75	108)
(76	7)	(77	9)	(78	4)	(79	3)	(82	4)
(84	4)	(86	10)	(87	8)	(89	9)	(90	7)
(91	17)	(100	198)	(101	26)	(102	12)	(103	15)
(104	4)	(105	10)	(115	9)	(116	4)	(117	14)
(118	8)	(119	9)	(130	22)	(131	30)	(132	26)

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(133	32)	(134	7)	(135	11)	(144	3)	(145	4)
(146	11)	(147	267)	(148	47)	(149	41)	(150	6)
(151	5)	(158	3)	(159	3)	(160	7)	(161	5)
(162	3)	(163	22)	(164	8)	(165	12)	(174	7)
(175	5)	(176	7)	(177	7)	(179	122)	(180	28)
(181	8)	(190	5)	(192	16)	(193	6)	(203	5)
(207	7)	(208	7)	(218	883)	(219	179)	(220	79)
(221	10)	(223	3)	(265	9)	(266	3)	(279	4)
(280	68)	(281	18)	(282	6)	(292	3)	(354	14)
(355	7)	(356	4)	(382	8)	(383	3)		

NAME:12C_2023.7_1274EC17_[680; Glycerol-2-phosphate (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203004-10-1

RI:2024

RT:13.138

NUM PEAKS: 93

(70	7)	(72	22)	(73	1000)	(74	84)	(75	188)
(76	13)	(77	20)	(86	5)	(88	14)	(89	11)
(90	3)	(95	16)	(99	11)	(101	15)	(103	22)
(105	7)	(111	10)	(113	15)	(114	4)	(115	13)
(121	5)	(125	4)	(126	5)	(127	11)	(130	8)
(131	16)	(133	86)	(134	11)	(135	23)	(137	12)
(141	9)	(142	10)	(143	11)	(147	254)	(148	39)
(149	32)	(150	5)	(151	6)	(153	10)	(155	11)
(160	7)	(161	5)	(163	3)	(167	9)	(168	11)
(169	138)	(170	24)	(171	22)	(177	3)	(179	9)
(181	11)	(183	8)	(184	27)	(185	9)	(186	3)
(193	10)	(195	12)	(197	3)	(198	4)	(200	5)
(207	14)	(208	5)	(211	102)	(212	19)	(213	9)
(215	9)	(225	13)	(227	34)	(228	7)	(229	4)
(241	7)	(242	3)	(243	203)	(244	46)	(245	23)
(253	7)	(256	3)	(257	7)	(258	115)	(259	32)
(260	13)	(285	4)	(297	58)	(298	14)	(299	107)
(300	31)	(301	16)	(302	4)	(315	93)	(316	25)
(317	11)	(370	4)	(485	5)				

NAME:12C_2029.2_1274EC17_[910; 9-(Z)-Hexadecenoic acid (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:203002-10-1

RI:2029

RT:13.173

NUM PEAKS: 136

(70	37)	(71	26)	(72	39)	(73	715)	(74	83)
(75	1000)	(76	70)	(77	71)	(78	12)	(79	85)
(80	34)	(81	177)	(82	84)	(83	121)	(84	171)
(85	34)	(86	11)	(87	6)	(88	5)	(89	25)
(90	3)	(91	37)	(92	12)	(93	53)	(94	30)
(95	124)	(96	197)	(97	108)	(98	143)	(99	33)
(100	3)	(101	10)	(102	6)	(103	3)	(105	33)
(106	7)	(107	26)	(108	18)	(109	64)	(110	74)
(111	48)	(112	29)	(113	7)	(115	6)	(116	60)
(117	697)	(118	68)	(119	52)	(120	8)	(121	30)
(122	12)	(123	52)	(124	32)	(125	16)	(126	6)
(127	7)	(128	5)	(129	533)	(130	66)	(131	109)
(132	124)	(133	44)	(134	26)	(135	19)	(136	9)
(137	39)	(138	33)	(139	13)	(140	4)	(141	14)
(142	6)	(143	36)	(144	7)	(145	211)	(146	28)
(148	11)	(149	6)	(150	4)	(151	24)	(152	70)
(153	13)	(154	4)	(155	29)	(156	9)	(157	16)

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(158	7)	(159	18)	(161	7)	(162	4)	(163	4)
(165	14)	(166	13)	(167	4)	(169	3)	(170	6)
(171	25)	(172	10)	(173	12)	(174	4)	(175	3)
(179	6)	(180	5)	(183	16)	(185	49)	(186	12)
(187	10)	(188	5)	(192	9)	(193	11)	(194	48)
(195	7)	(199	62)	(200	12)	(201	12)	(202	3)
(207	4)	(208	7)	(213	12)	(214	3)	(215	4)
(218	3)	(227	7)	(229	8)	(230	3)	(236	32)
(237	7)	(241	4)	(255	3)	(267	4)	(283	4)
(310	4)	(311	136)	(312	39)	(313	9)	(326	15)
(327	5)								

NAME:12C_1675.0_1274EC11_[877; Pyrophosphoric acid (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:168004-10-1

RI:1675

RT:10.627

NUM PEAKS: 96

(70	7)	(71	12)	(72	46)	(73	1000)	(74	92)
(75	44)	(83	12)	(85	8)	(87	3)	(89	6)
(91	4)	(95	6)	(97	7)	(98	3)	(99	5)
(100	6)	(103	21)	(104	5)	(107	5)	(111	4)
(114	3)	(115	9)	(119	10)	(121	14)	(125	3)
(127	21)	(131	6)	(133	61)	(134	7)	(135	43)
(136	4)	(137	11)	(139	4)	(146	13)	(151	9)
(165	8)	(167	5)	(177	5)	(179	5)	(180	3)
(181	10)	(187	3)	(189	5)	(191	24)	(192	7)
(193	48)	(194	7)	(195	28)	(196	4)	(197	6)
(205	5)	(207	57)	(208	12)	(209	10)	(211	10)
(212	3)	(217	17)	(218	5)	(225	13)	(226	3)
(230	3)	(254	3)	(255	7)	(257	4)	(267	3)
(269	12)	(270	3)	(273	3)	(283	16)	(284	6)
(285	26)	(286	6)	(297	4)	(299	74)	(300	18)
(301	8)	(313	6)	(314	7)	(315	3)	(362	3)
(363	24)	(364	7)	(365	4)	(435	4)	(436	4)
(449	5)	(450	55)	(451	369)	(452	150)	(453	80)
(454	21)	(455	6)	(465	5)	(466	35)	(467	15)
(468	9)								

NAME:12C_1673.8_1191EC10_Homocysteine (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:167001-10-1

RI:1674

RT:10.561

NUM PEAKS: 223

(70	16)	(72	171)	(75	990)	(76	88)	(77	1000)
(78	54)	(79	20)	(82	133)	(84	120)	(88	18)
(89	233)	(90	28)	(91	61)	(92	38)	(93	136)
(94	11)	(95	104)	(97	29)	(98	463)	(99	39)
(101	48)	(102	26)	(103	326)	(104	38)	(105	44)
(106	5)	(107	10)	(111	21)	(114	105)	(119	83)
(120	9)	(121	19)	(122	13)	(124	16)	(125	15)
(127	136)	(128	510)	(129	16)	(130	63)	(137	15)
(139	17)	(142	13)	(144	40)	(146	159)	(155	29)
(156	89)	(157	39)	(161	5)	(162	23)	(165	19)
(166	4)	(167	8)	(171	49)	(176	6)	(183	14)
(184	22)	(185	22)	(187	33)	(193	22)	(200	14)
(201	4)	(202	21)	(203	14)	(212	21)	(214	5)
(224	6)	(228	4)	(229	18)	(230	19)	(234	191)
(235	42)	(236	18)	(241	5)	(244	12)	(250	10)

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(257	10)	(261	10)	(262	14)	(265	6)	(266	7)
(267	7)	(268	23)	(271	30)	(280	5)	(281	4)
(283	11)	(291	4)	(293	4)	(294	6)	(295	10)
(298	6)	(308	19)	(309	4)	(312	5)	(314	38)
(315	12)	(316	17)	(318	9)	(319	18)	(320	9)
(322	12)	(325	10)	(334	19)	(335	8)	(337	16)
(338	7)	(340	10)	(345	10)	(346	22)	(348	6)
(349	4)	(350	17)	(351	14)	(352	9)	(353	8)
(368	4)	(370	9)	(371	13)	(372	5)	(381	5)
(383	10)	(384	4)	(386	4)	(388	5)	(391	6)
(392	10)	(393	10)	(394	12)	(395	15)	(396	3)
(399	3)	(401	7)	(402	6)	(403	5)	(416	6)
(417	5)	(418	11)	(423	6)	(427	6)	(431	7)
(432	13)	(433	7)	(434	6)	(435	6)	(438	11)
(442	5)	(444	9)	(445	11)	(446	6)	(448	8)
(456	5)	(457	16)	(458	12)	(459	7)	(460	7)
(461	10)	(464	14)	(471	4)	(472	10)	(473	10)
(475	5)	(476	5)	(477	4)	(478	18)	(480	6)
(481	7)	(482	3)	(483	16)	(487	12)	(488	4)
(491	17)	(492	12)	(494	8)	(495	11)	(496	4)
(497	4)	(498	7)	(500	8)	(501	10)	(502	9)
(504	8)	(505	19)	(510	8)	(511	5)	(512	6)
(514	4)	(515	8)	(517	13)	(518	3)	(520	8)
(521	16)	(522	10)	(523	4)	(525	6)	(526	5)
(527	6)	(528	10)	(532	7)	(533	6)	(535	7)
(536	8)	(539	7)	(546	6)	(547	7)	(549	3)
(550	5)	(551	7)	(553	6)	(554	7)	(555	10)
(556	3)	(557	6)	(559	4)	(563	5)	(566	4)
(567	7)	(568	7)	(573	6)	(575	3)	(576	3)
(581	5)	(585	3)	(593	3)				

NAME:12C_1522.3_1313EC36_Methionine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:152001-10-1

RI:1522

RT:8.924

NUM PEAKS: -108

(73	999)	(78	21)	(79	29)	(93	23)	(108	5)
(122	4)	(128	997)	(129	132)	(166	10)	(176	1000)
(177	142)	(178	78)	(182	7)	(209	8)	(225	7)
(226	9)	(229	7)	(238	8)	(241	3)	(249	5)
(250	53)	(251	13)	(252	7)	(269	8)	(270	6)
(288	6)	(290	10)	(293	55)	(295	12)	(297	5)
(298	8)	(300	4)	(303	3)	(312	6)	(313	10)
(314	4)	(315	8)	(317	4)	(324	3)	(345	8)
(354	7)	(367	5)	(368	8)	(369	6)	(370	4)
(371	8)	(374	6)	(379	5)	(380	3)	(381	9)
(382	6)	(383	7)	(386	4)	(387	5)	(388	9)
(389	4)	(398	6)	(400	3)	(404	3)	(405	3)
(406	7)	(410	4)	(419	5)	(420	5)	(421	9)
(423	3)	(424	4)	(426	6)	(432	4)	(433	7)
(434	7)	(435	4)	(439	5)	(444	6)	(452	8)
(457	6)	(461	7)	(462	10)	(466	4)	(467	6)
(472	5)	(478	6)	(479	5)	(480	4)	(484	7)
(485	7)	(489	4)	(491	4)	(492	5)	(493	4)
(496	4)	(497	7)	(500	7)	(501	4)	(509	5)
(513	5)	(516	3)	(517	4)	(520	3)	(524	4)
(526	6)	(532	4)	(544	5)	(545	3)	(548	10)
(555	5)	(559	4)	(560	4)				

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NAME:12C_1560.7_1191EC08_Cysteine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:156002-10-1
RI:1561

RT:9.691

NUM PEAKS: 49

(72	25)	(73	1000)	(74	66)	(75	68)	(86	15)
(89	7)	(95	3)	(98	3)	(99	3)	(100	171)
(101	25)	(102	5)	(105	9)	(114	5)	(115	20)
(116	44)	(117	28)	(129	9)	(131	9)	(132	60)
(133	32)	(134	8)	(138	4)	(144	5)	(147	94)
(148	30)	(149	14)	(155	10)	(158	4)	(159	3)
(163	4)	(174	28)	(203	4)	(204	6)	(205	3)
(212	3)	(218	166)	(219	33)	(220	184)	(221	40)
(222	22)	(232	5)	(243	3)	(246	3)	(247	4)
(257	3)	(294	7)	(295	3)	(322	3)		

NAME:12C_1281.5_1313EC36_Ethanolamine (3TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1282 |RI:1282
CASNO:128002-10-1

RI:1282

RT:6.152

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 25

(72	19)	(73	1000)	(74	79)	(75	133)	(86	276)
(87	20)	(88	19)	(100	284)	(101	33)	(102	25)
(103	26)	(114	30)	(117	30)	(130	53)	(131	45)
(133	83)	(134	8)	(144	24)	(148	14)	(158	7)
(172	10)	(174	945)	(175	165)	(176	57)	(188	8)

NAME:12C_1364.2_1313EC11_Uracil (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:136001-10-1

RI:1364

RT:7.160

NUM PEAKS: 30

(72	155)	(73	836)	(74	77)	(86	38)	(96	27)
(98	37)	(99	1000)	(100	270)	(101	91)	(103	22)
(105	25)	(109	39)	(113	231)	(114	21)	(117	37)
(126	260)	(127	37)	(131	109)	(133	50)	(147	605)
(148	91)	(153	26)	(169	32)	(239	24)	(241	624)
(242	130)	(243	43)	(255	318)	(256	270)	(257	64)

NAME:12C_1372.9_1313EC75_Fumaric acid (2TMS)
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
CASNO:137001-10-1

RI:1373

RT:7.260

NUM PEAKS: 37

(72	44)	(73	1000)	(74	116)	(75	637)	(77	32)
(80	12)	(82	49)	(83	207)	(84	81)	(111	12)
(112	19)	(115	105)	(117	23)	(127	62)	(128	21)
(133	150)	(134	22)	(135	32)	(143	183)	(144	26)
(147	940)	(148	150)	(149	114)	(155	73)	(156	29)
(157	37)	(171	21)	(184	23)	(199	16)	(207	20)
(215	16)	(217	43)	(242	12)	(245	650)	(246	139)
(247	70)	(259	29)						

NAME:12C_1450.0_1313EC75_[690; N,N-Di-(2-Hydroxyethyl)-methanamine (2TMS)]
COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

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CASNO:144007-10-1

RI:1450

RT:8.1600

NUM PEAKS: 162

(70	5)	(71	5)	(72	37)	(73	1000)	(74	118)
(75	311)	(76	37)	(77	19)	(81	2)	(83	1)
(84	3)	(87	19)	(89	20)	(90	2)	(91	3)
(92	3)	(93	1)	(97	5)	(98	3)	(100	46)
(101	17)	(102	17)	(103	30)	(104	8)	(105	12)
(110	4)	(114	7)	(115	25)	(116	110)	(117	232)
(118	25)	(119	26)	(120	3)	(122	1)	(123	2)
(125	9)	(128	15)	(129	5)	(130	164)	(131	56)
(132	18)	(133	43)	(134	6)	(135	4)	(136	2)
(137	4)	(143	1)	(144	27)	(146	12)	(147	128)
(148	23)	(149	26)	(150	5)	(151	6)	(154	10)
(157	21)	(158	6)	(159	11)	(160	270)	(161	38)
(162	6)	(163	43)	(164	7)	(165	3)	(169	2)
(170	6)	(172	8)	(174	2)	(175	9)	(177	1)
(180	3)	(185	1)	(187	1)	(188	4)	(189	3)
(200	1)	(201	10)	(202	5)	(204	1)	(205	8)
(207	2)	(211	6)	(212	6)	(215	7)	(217	2)
(220	3)	(221	1)	(228	2)	(232	7)	(234	9)
(236	5)	(245	19)	(246	6)	(247	5)	(248	5)
(253	2)	(254	3)	(256	1)	(257	2)	(260	3)
(262	7)	(264	3)	(277	2)	(278	6)	(287	3)
(288	4)	(290	2)	(300	2)	(301	5)	(302	7)
(308	1)	(319	1)	(320	9)	(321	3)	(322	4)
(335	1)	(336	2)	(353	4)	(354	4)	(369	3)
(376	2)	(387	3)	(404	1)	(407	1)	(410	5)
(411	2)	(415	3)	(421	3)	(422	5)	(427	6)
(430	3)	(435	3)	(438	3)	(441	2)	(449	1)
(464	3)	(467	3)	(469	7)	(470	4)	(474	2)
(477	4)	(484	1)	(487	1)	(494	4)	(500	1)
(501	2)	(503	2)	(510	2)	(511	1)	(516	1)
(517	4)	(519	2)	(520	1)	(522	6)	(524	1)
(533	6)	(536	1)	(540	2)	(541	3)	(543	1)
(552	7)	(564	1)						

NAME:12C_1503.9_1313EC75_Erythritol (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:150002-10-1

RI:1504

RT:8.781

NUM PEAKS: 181

(73	1000)	(74	80)	(75	187)	(76	14)	(87	6)
(88	6)	(89	68)	(90	5)	(101	43)	(103	155)
(104	15)	(105	11)	(115	37)	(116	51)	(117	136)
(118	12)	(119	13)	(120	3)	(122	2)	(129	53)
(130	4)	(131	38)	(132	4)	(133	87)	(134	11)
(135	10)	(143	28)	(144	3)	(145	9)	(147	338)
(148	51)	(149	35)	(150	4)	(151	3)	(157	10)
(158	3)	(161	5)	(162	2)	(163	14)	(164	3)
(171	7)	(173	6)	(174	3)	(175	10)	(177	5)
(178	2)	(185	4)	(187	5)	(188	2)	(189	56)
(190	11)	(191	40)	(192	8)	(193	3)	(195	2)
(198	2)	(199	4)	(201	21)	(202	3)	(203	13)
(204	53)	(205	90)	(206	19)	(207	9)	(209	5)
(215	7)	(216	3)	(217	173)	(218	35)	(219	13)
(221	9)	(222	5)	(229	6)	(230	3)	(231	11)
(233	2)	(238	3)	(240	2)	(244	2)	(247	5)

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(248	4)	(249	3)	(251	2)	(259	5)	(260	3)
(263	1)	(264	2)	(265	2)	(266	2)	(274	2)
(275	19)	(276	6)	(277	8)	(278	3)	(279	2)
(280	3)	(281	2)	(285	2)	(286	3)	(287	2)
(288	2)	(289	3)	(290	3)	(291	8)	(292	3)
(293	14)	(294	5)	(305	4)	(306	3)	(307	13)
(308	4)	(311	2)	(312	3)	(316	2)	(319	7)
(320	6)	(321	3)	(322	2)	(325	2)	(326	3)
(327	2)	(328	3)	(334	2)	(335	2)	(336	3)
(337	2)	(342	2)	(347	2)	(349	2)	(353	4)
(361	2)	(372	2)	(373	2)	(374	3)	(376	2)
(382	2)	(391	3)	(400	2)	(409	3)	(415	1)
(419	2)	(420	2)	(424	2)	(428	3)	(429	2)
(433	2)	(435	2)	(440	2)	(442	3)	(447	2)
(454	2)	(455	2)	(456	2)	(457	2)	(458	2)
(459	1)	(462	2)	(463	3)	(476	1)	(478	2)
(482	2)	(484	2)	(492	2)	(493	2)	(495	2)
(501	2)	(506	3)	(507	3)	(516	3)	(522	2)
(523	2)	(529	2)	(532	3)	(537	2)	(539	2)
(540	2)	(544	2)	(552	1)	(564	2)	(571	2)
(575	2)								

NAME:12C_1694.8_1313EC75_[746; Ribonic acid-1,4-lactone (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:169001-10-1

RI:1695

RT:10.265

NUM PEAKS: 27

(73	1000)	(74	77)	(75	69)	(101	36)	(102	70)
(117	211)	(130	64)	(133	105)	(139	7)	(143	14)
(147	260)	(148	31)	(149	56)	(153	6)	(189	23)
(191	21)	(203	14)	(215	54)	(217	23)	(231	32)
(246	25)	(248	16)	(259	33)	(349	16)	(355	7)
(413	11)	(564	11)						

NAME:12C_1670.8_1313EC75_Arabinose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer [RI:1671 [RI:1671 [RI:1671

CASNO:167002-10-1

RI:1671

RT:10.078

SOURCE:C:\KOPKA\AMDIS32\LIB\File2.msp

NUM PEAKS: 142

(70	8)	(71	6)	(72	22)	(73	1000)	(74	88)
(75	83)	(76	4)	(82	3)	(83	3)	(84	4)
(85	7)	(86	6)	(87	8)	(88	5)	(89	56)
(90	5)	(96	1)	(99	6)	(100	27)	(101	23)
(102	10)	(103	397)	(104	37)	(105	31)	(111	2)
(112	2)	(113	5)	(114	8)	(115	9)	(116	8)
(117	43)	(118	4)	(119	8)	(125	1)	(126	2)
(127	3)	(128	4)	(129	52)	(130	11)	(131	35)
(132	5)	(133	68)	(134	8)	(136	1)	(140	2)
(141	1)	(142	5)	(143	14)	(144	3)	(145	7)
(146	1)	(147	200)	(148	31)	(149	21)	(150	2)
(151	1)	(152	1)	(154	1)	(156	1)	(157	3)
(158	5)	(159	3)	(160	40)	(161	10)	(162	2)
(163	8)	(164	1)	(165	1)	(168	9)	(169	2)
(170	4)	(171	1)	(172	6)	(173	5)	(174	7)
(175	6)	(176	1)	(177	3)	(184	1)	(186	1)
(187	1)	(188	1)	(189	44)	(190	15)	(191	16)
(192	3)	(193	1)	(198	3)	(199	1)	(200	2)

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(201	3)	(203	3)	(204	18)	(205	21)	(206	4)
(207	3)	(216	5)	(217	199)	(218	41)	(219	18)
(220	2)	(221	5)	(222	1)	(223	1)	(228	1)
(230	1)	(231	3)	(232	2)	(233	15)	(234	6)
(235	1)	(240	1)	(242	3)	(243	1)	(244	1)
(248	2)	(250	1)	(256	3)	(257	2)	(258	5)
(259	1)	(260	1)	(262	5)	(263	1)	(272	1)
(274	2)	(276	1)	(277	15)	(278	5)	(279	2)
(291	3)	(292	1)	(306	3)	(307	65)	(308	19)
(309	9)	(310	1)	(330	1)	(331	1)	(332	1)
(361	1)	(362	1)						

NAME:12C_1726.7_1313EC36_Fucose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:173002-10-1

RI:1727

RT:10.513

NUM PEAKS: 58

(72	15)	(73	1000)	(74	73)	(75	131)	(83	25)
(101	11)	(103	84)	(104	13)	(105	105)	(106	11)
(115	16)	(117	495)	(118	44)	(119	15)	(131	35)
(133	70)	(147	257)	(148	47)	(149	35)	(157	19)
(158	12)	(174	29)	(176	7)	(187	14)	(190	23)
(191	19)	(203	14)	(204	13)	(205	30)	(209	11)
(211	8)	(217	99)	(218	12)	(231	12)	(242	6)
(245	39)	(246	71)	(247	11)	(255	7)	(263	6)
(267	7)	(268	11)	(276	7)	(299	7)	(318	8)
(319	19)	(320	13)	(321	7)	(378	11)	(380	9)
(407	8)	(410	7)	(437	7)	(444	10)	(493	7)
(504	8)	(519	8)	(555	6)				

NAME:12C_1784.9_1313EC75_[798; Ribonic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:179001-10-1

RI:1785

RT:10.966

NUM PEAKS: 44

(72	16)	(73	1000)	(74	81)	(75	50)	(89	17)
(101	13)	(102	19)	(103	207)	(104	18)	(105	8)
(117	50)	(119	6)	(130	17)	(131	26)	(132	6)
(133	76)	(134	8)	(143	28)	(145	4)	(147	282)
(148	38)	(175	5)	(189	38)	(190	7)	(191	16)
(205	33)	(206	6)	(207	7)	(217	134)	(218	24)
(219	16)	(221	15)	(222	5)	(257	7)	(277	15)
(278	6)	(292	128)	(293	38)	(294	16)	(305	19)
(306	7)	(307	18)	(331	7)	(333	15)		

NAME:12C_1806.2_1313EC75_[549; 2-Keto-D-gluconic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:181004-10-1

RI:1806

RT:11.131

NUM PEAKS: 57

(73	1000)	(74	98)	(90	8)	(102	16)	(128	11)
(131	24)	(133	40)	(134	12)	(147	160)	(159	17)
(161	12)	(162	12)	(187	131)	(188	28)	(213	15)
(215	18)	(217	126)	(218	33)	(219	23)	(245	8)
(246	10)	(254	9)	(257	56)	(265	6)	(266	11)
(268	8)	(280	9)	(285	9)	(302	9)	(303	14)
(304	8)	(313	11)	(327	12)	(352	11)	(363	11)

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(365 13) (369 8) (399 11) (400 8) (401 9)
 (410 7) (437 37) (441 10) (475 11) (488 13)
 (494 14) (498 11) (499 14) (510 10) (522 10)
 (528 15) (536 15) (555 8) (563 8) (573 4)
 (593 2) (599 2)

NAME:12C_1842.1_1313EC75_[693; 2-Furan-2-hydroxyacetic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:184002-10-1

RI:1842

RT:11.411

NUM PEAKS: 122

(70 8) (71 7) (72 21) (73 1000) (74 90)
 (75 144) (76 10) (77 12) (78 1) (79 4)
 (80 12) (81 83) (82 6) (83 7) (85 11)
 (87 5) (88 4) (89 13) (92 2) (93 11)
 (94 7) (95 46) (96 11) (97 14) (98 19)
 (99 11) (100 5) (101 41) (106 2) (107 8)
 (108 2) (109 4) (110 3) (111 4) (112 11)
 (113 3) (115 6) (117 96) (118 7) (119 15)
 (121 5) (122 1) (123 6) (124 4) (125 12)
 (126 7) (127 8) (131 23) (132 5) (133 65)
 (134 10) (135 7) (137 5) (138 23) (139 13)
 (140 7) (147 191) (148 28) (149 19) (150 2)
 (151 7) (152 4) (153 49) (154 49) (155 19)
 (166 23) (167 55) (168 11) (169 860) (170 497)
 (171 86) (172 14) (175 5) (179 8) (180 1)
 (181 5) (182 8) (183 4) (193 2) (194 10)
 (195 23) (196 3) (197 2) (199 2) (205 18)
 (206 3) (207 2) (209 1) (210 10) (211 3)
 (212 3) (227 2) (239 10) (240 3) (241 28)
 (242 43) (243 14) (255 5) (256 2) (257 2)
 (267 1) (268 2) (269 17) (270 6) (271 4)
 (283 3) (284 26) (285 4) (286 2) (313 1)
 (329 12) (330 4) (331 2) (358 2) (359 13)
 (360 3) (373 1) (374 20) (375 7) (376 4)
 (377 1) (390 1)

NAME:12C_1848.6_1313EC75_[708; Glucose methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:185003-10-1

RI:1849

RT:11.461

NUM PEAKS: 137

(70 4) (71 6) (72 18) (73 1000) (74 86)
 (75 120) (76 7) (77 6) (82 10) (83 4)
 (84 2) (85 8) (86 4) (87 6) (88 4)
 (89 83) (90 7) (91 4) (92 1) (94 1)
 (99 5) (100 16) (101 20) (102 8) (103 195)
 (104 20) (105 19) (106 3) (111 4) (112 2)
 (113 4) (114 4) (115 8) (117 71) (118 6)
 (119 9) (120 1) (126 3) (127 5) (129 104)
 (130 44) (131 23) (133 65) (134 8) (135 6)
 (141 2) (142 7) (143 13) (144 2) (145 9)
 (146 2) (147 109) (148 18) (149 21) (150 3)
 (151 2) (152 1) (157 195) (158 29) (159 13)
 (160 47) (161 44) (162 7) (163 48) (164 8)
 (165 4) (168 1) (172 4) (174 6) (175 4)
 (176 1) (177 5) (178 1) (180 2) (182 1)
 (186 2) (187 2) (188 2) (189 77) (190 15)

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(191	14)	(192	2)	(193	1)	(196	1)	(198	1)
(200	1)	(202	1)	(203	7)	(204	11)	(205	49)
(206	10)	(212	1)	(214	5)	(215	3)	(216	3)
(217	47)	(218	16)	(219	15)	(220	3)	(228	2)
(229	11)	(230	5)	(231	9)	(232	4)	(233	10)
(234	2)	(235	7)	(236	1)	(237	1)	(240	1)
(243	4)	(244	50)	(245	13)	(246	7)	(247	30)
(248	7)	(249	3)	(259	3)	(260	1)	(261	1)
(262	1)	(268	1)	(270	2)	(274	1)	(275	1)
(276	1)	(278	1)	(291	1)	(302	2)	(304	2)
(305	1)	(319	27)	(320	9)	(321	4)	(322	1)
(333	1)	(337	1)						

NAME:12C_2113.2_1313EC36_1697; Ribose-5-phosphate methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211003-10-1

RT:2113

RT:13.210

NUM PEAKS: 16

(73	1000)	(74	94)	(89	45)	(129	96)	(133	74)
(147	155)	(157	20)	(207	19)	(211	57)	(217	123)
(299	117)	(300	41)	(315	157)	(316	50)	(317	31)
(459	18)								

NAME:12C_2225.2_1313EC36_Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223003-10-1

RI:2225

RT:13.896

NUM PEAKS: 126

(70	45)	(71	28)	(72	42)	(73	1000)	(75	767)
(76	50)	(77	44)	(80	13)	(81	109)	(82	71)
(83	95)	(84	111)	(85	25)	(86	17)	(88	12)
(89	20)	(94	22)	(95	93)	(96	137)	(97	82)
(98	100)	(99	27)	(100	47)	(101	29)	(102	26)
(107	11)	(108	14)	(109	47)	(110	50)	(111	31)
(112	22)	(113	12)	(114	8)	(116	57)	(117	394)
(118	37)	(119	33)	(121	14)	(122	11)	(123	37)
(124	28)	(125	16)	(126	7)	(128	9)	(129	376)
(130	65)	(131	77)	(132	115)	(137	14)	(138	20)
(139	11)	(143	22)	(144	10)	(145	146)	(146	21)
(149	12)	(151	7)	(152	23)	(153	6)	(155	11)
(158	12)	(159	15)	(162	6)	(166	17)	(170	15)
(171	19)	(172	14)	(173	15)	(180	23)	(183	11)
(184	9)	(185	39)	(186	18)	(187	10)	(188	12)
(190	12)	(199	35)	(200	28)	(208	7)	(210	4)
(214	7)	(218	26)	(220	13)	(222	23)	(235	8)
(240	6)	(248	8)	(264	21)	(268	4)	(272	5)
(274	7)	(275	8)	(283	5)	(303	8)	(309	6)
(337	10)	(338	8)	(339	75)	(340	28)	(354	8)
(362	7)	(363	7)	(378	4)	(385	5)	(407	11)
(412	8)	(413	7)	(446	6)	(449	8)	(454	4)
(456	6)	(459	4)	(471	6)	(472	10)	(475	11)
(480	9)	(486	4)	(487	5)	(513	6)	(520	5)
(521	7)	(527	5)	(550	4)	(568	6)	(586	4)
(588	4)								

NAME:12C_3270.3_1313EC36_Ergosterol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:327001-10-1

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RI:3270

RT:19.000

NUM PEAKS: 189

(70	153)	(71	80)	(72	19)	(73	1000)	(74	107)
(75	502)	(76	64)	(77	163)	(78	39)	(79	251)
(80	30)	(81	452)	(82	78)	(83	274)	(84	26)
(85	27)	(86	10)	(87	18)	(88	9)	(89	43)
(90	11)	(91	309)	(92	39)	(93	193)	(94	32)
(95	188)	(96	24)	(97	81)	(98	15)	(99	12)
(101	30)	(102	19)	(103	43)	(104	19)	(105	224)
(106	27)	(107	133)	(108	21)	(109	130)	(110	16)
(111	33)	(113	10)	(114	4)	(115	190)	(116	50)
(117	140)	(118	44)	(119	323)	(120	38)	(121	55)
(122	8)	(123	47)	(124	9)	(125	88)	(126	18)
(127	57)	(128	242)	(129	373)	(130	87)	(131	429)
(132	69)	(133	92)	(134	14)	(135	42)	(136	8)
(137	28)	(138	5)	(139	17)	(140	6)	(141	222)
(142	142)	(143	453)	(144	272)	(145	294)	(146	57)
(147	74)	(148	11)	(149	27)	(150	9)	(151	22)
(152	55)	(153	88)	(154	60)	(155	217)	(156	88)
(157	392)	(158	128)	(159	234)	(160	41)	(161	19)
(162	5)	(163	21)	(164	11)	(165	89)	(166	43)
(167	80)	(168	64)	(169	224)	(170	80)	(171	165)
(172	41)	(173	43)	(174	9)	(175	10)	(176	6)
(177	8)	(178	26)	(179	40)	(180	24)	(181	85)
(182	60)	(183	169)	(184	53)	(185	129)	(186	31)
(187	18)	(188	4)	(189	9)	(191	11)	(192	7)
(193	22)	(194	25)	(196	51)	(197	165)	(198	57)
(199	111)	(200	23)	(201	22)	(202	7)	(205	10)
(206	5)	(207	13)	(208	8)	(209	58)	(211	228)
(212	60)	(213	83)	(214	16)	(215	7)	(219	7)
(223	39)	(224	19)	(225	49)	(226	53)	(227	43)
(228	9)	(229	5)	(238	29)	(239	55)	(240	14)
(241	6)	(247	3)	(248	3)	(251	68)	(252	33)
(253	164)	(254	37)	(255	6)	(265	21)	(266	7)
(267	13)	(268	4)	(279	12)	(280	12)	(281	8)
(293	13)	(294	6)	(295	4)	(310	5)	(323	5)
(326	10)	(327	6)	(335	6)	(336	17)	(337	227)
(338	82)	(339	18)	(343	6)	(363	317)	(364	119)
(365	21)	(377	14)	(378	79)	(379	31)	(380	5)
(467	9)	(468	53)	(469	28)	(470	8)		

NAME:12C_1580.7_1313EC75_[829; 1-Phenylethanol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:158002-10-1

RI:1581

RT:9.378

NUM PEAKS: 10

(82	34)	(179	1000)	(180	165)	(181	44)	(193	105)
(194	19)	(267	71)	(268	15)	(269	6)	(284	6)

NAME:12C_2109.7_1313EC75_[662; Ribose-5-phosphate methoxyamine {BP} (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:211004-10-1

RI:2110

RT:13.188

NUM PEAKS: 47

(72	27)	(73	1000)	(74	90)	(75	151)	(77	24)
(89	42)	(98	13)	(100	40)	(101	45)	(104	8)
(105	22)	(114	12)	(115	15)	(117	75)	(119	14)

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(129 122) (130 31) (131 42) (132 33) (133 69)
 (135 24) (138 7) (143 14) (145 21) (147 232)
 (158 31) (160 40) (175 5) (189 17) (191 16)
 (195 10) (207 13) (211 46) (212 13) (217 118)
 (218 29) (219 10) (225 13) (299 96) (300 31)
 (301 13) (315 143) (316 39) (321 8) (357 16)
 (387 9) (403 14)

NAME:12C_2125.3_1313EC75_[832; Dopamine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213003-10-1

RI:2125

RT:13.287

NUM PEAKS: 53

(72 18) (73 816) (74 58) (75 62) (77 7)
 (86 118) (89 9) (96 5) (100 38) (102 20)
 (103 20) (104 14) (114 9) (115 9) (117 58)
 (128 12) (130 23) (131 27) (133 29) (139 7)
 (143 13) (147 282) (148 40) (161 8) (172 13)
 (174 1000) (175 190) (176 68) (177 6) (178 7)
 (188 8) (189 19) (204 17) (205 21) (207 5)
 (216 7) (217 26) (218 9) (248 4) (259 9)
 (288 5) (290 17) (291 12) (299 6) (304 9)
 (307 10) (344 5) (355 5) (396 6) (443 5)
 (475 4) (591 4) (599 3)

NAME:12C_2155.6_1313EC75_[795; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216003-10-1

RI:2156

RT:13.479

NUM PEAKS: 106

(72 14) (73 1000) (74 86) (80 5) (84 7)
 (86 10) (88 22) (93 3) (94 3) (100 6)
 (103 163) (104 18) (105 12) (107 4) (108 3)
 (114 7) (116 19) (117 86) (118 9) (119 7)
 (127 5) (128 7) (129 46) (130 17) (131 16)
 (132 4) (133 46) (134 7) (135 5) (140 4)
 (141 6) (142 26) (143 15) (144 12) (145 3)
 (146 26) (147 239) (148 36) (149 27) (150 3)
 (151 3) (155 4) (157 27) (158 14) (163 3)
 (168 9) (169 9) (172 7) (173 16) (174 43)
 (175 7) (179 3) (180 4) (181 3) (184 3)
 (189 20) (191 12) (196 3) (197 14) (198 7)
 (200 11) (201 4) (202 3) (203 5) (204 17)
 (205 60) (206 14) (207 9) (216 4) (217 77)
 (218 19) (219 6) (221 12) (228 4) (229 25)
 (230 6) (231 3) (232 4) (243 9) (256 7)
 (257 7) (259 3) (269 4) (311 5) (313 4)
 (314 11) (315 7) (319 8) (320 3) (339 6)
 (343 4) (344 5) (345 26) (346 9) (347 4)
 (357 6) (370 5) (371 4) (375 5) (429 6)
 (433 3) (435 3) (519 10) (520 3) (521 3)
 (523 3)

NAME:12C_2162.3_1313EC75_[648; Ethylamine (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:216002-10-1

RI:2162

RT:13.521

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NUM PEAKS: 54

(72	18)	(73	1000)	(74	79)	(75	51)	(86	127)
(87	17)	(89	31)	(100	88)	(101	23)	(102	17)
(103	161)	(104	15)	(106	4)	(115	7)	(117	64)
(118	9)	(129	34)	(130	20)	(132	6)	(133	39)
(134	6)	(143	9)	(157	10)	(172	25)	(173	9)
(174	283)	(175	54)	(176	20)	(185	12)	(189	17)
(190	8)	(199	5)	(200	4)	(204	13)	(205	45)
(206	10)	(207	5)	(216	10)	(217	93)	(218	19)
(219	9)	(231	4)	(241	16)	(259	6)	(267	7)
(272	16)	(287	15)	(288	6)	(305	7)	(306	3)
(307	15)	(314	11)	(315	12)	(346	5)		

NAME:12C_2168.9_1313EC75_[705; 2-Ketogluconic acid (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:217002-10-1

RI:2169

RT:13.563

NUM PEAKS: 52

(72	21)	(73	1000)	(74	81)	(75	70)	(79	5)
(86	63)	(87	12)	(89	11)	(100	35)	(102	10)
(103	35)	(115	6)	(116	5)	(117	26)	(129	37)
(130	16)	(131	28)	(133	34)	(134	9)	(141	30)
(142	8)	(145	4)	(147	269)	(148	43)	(149	25)
(150	5)	(156	5)	(157	17)	(167	4)	(170	4)
(172	8)	(174	104)	(175	22)	(176	8)	(189	16)
(191	41)	(192	8)	(205	17)	(207	7)	(215	11)
(217	47)	(218	13)	(257	45)	(258	12)	(303	12)
(304	7)	(319	12)	(425	3)	(436	9)	(437	40)
(438	20)	(439	9)						

NAME:12C_2180.5_1313EC75_[733; Threitol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:218001-10-1

RI:2181

RT:13.637

NUM PEAKS: 128

(70	7)	(72	20)	(73	1000)	(74	89)	(75	131)
(76	9)	(77	6)	(80	8)	(81	7)	(82	7)
(83	25)	(86	11)	(87	7)	(88	6)	(89	43)
(94	4)	(95	14)	(97	4)	(98	5)	(100	11)
(101	17)	(102	8)	(103	194)	(104	18)	(105	11)
(107	7)	(109	5)	(114	9)	(115	7)	(116	20)
(117	74)	(119	8)	(125	3)	(127	5)	(128	9)
(129	40)	(130	15)	(131	22)	(132	5)	(133	51)
(134	6)	(139	5)	(140	4)	(142	32)	(144	20)
(145	7)	(146	43)	(147	222)	(148	35)	(149	25)
(150	4)	(152	4)	(155	5)	(156	5)	(157	14)
(158	29)	(159	6)	(160	8)	(163	5)	(167	5)
(168	8)	(169	9)	(172	10)	(173	24)	(174	66)
(175	12)	(176	4)	(181	7)	(183	5)	(185	10)
(186	9)	(187	5)	(188	3)	(189	18)	(190	5)
(191	10)	(195	3)	(197	26)	(198	8)	(199	3)
(200	6)	(202	3)	(203	3)	(205	38)	(206	8)
(207	6)	(215	4)	(216	6)	(217	81)	(218	20)
(219	8)	(221	9)	(223	6)	(229	14)	(230	4)
(232	6)	(243	8)	(253	4)	(255	4)	(256	7)
(268	5)	(270	3)	(271	4)	(277	4)	(287	5)
(291	3)	(295	4)	(307	5)	(313	5)	(314	12)
(315	7)	(339	7)	(340	3)	(343	5)	(344	5)

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(345	40)	(346	12)	(347	4)	(370	5)	(371	3)
(375	6)	(429	6)	(430	3)	(433	4)	(518	3)
(519	8)	(523	8)	(524	4)				

NAME:12C_2245.5_1313EC75_Octadecanoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:225002-10-1

RI:2246

RT:14.001

NUM PEAKS: 124

(70	33)	(71	65)	(72	50)	(73	932)	(74	104)
(75	1000)	(76	73)	(77	57)	(78	3)	(79	29)
(80	4)	(81	78)	(82	12)	(83	87)	(84	26)
(85	39)	(86	13)	(88	7)	(89	29)	(90	5)
(91	13)	(92	3)	(93	27)	(94	4)	(95	69)
(96	12)	(97	66)	(98	48)	(99	28)	(100	4)
(101	15)	(102	6)	(105	28)	(106	3)	(107	14)
(109	22)	(110	4)	(111	32)	(112	14)	(113	6)
(115	10)	(116	65)	(117	947)	(118	94)	(119	39)
(121	11)	(123	7)	(125	9)	(126	4)	(127	6)
(128	4)	(129	493)	(130	64)	(131	162)	(132	487)
(133	105)	(134	25)	(135	12)	(137	3)	(139	5)
(140	4)	(141	5)	(143	51)	(144	7)	(145	282)
(146	39)	(149	5)	(151	3)	(153	5)	(154	9)
(155	7)	(157	15)	(158	3)	(159	33)	(160	6)
(163	3)	(167	4)	(168	3)	(171	28)	(172	4)
(173	8)	(174	4)	(185	44)	(186	7)	(187	25)
(188	9)	(199	12)	(201	76)	(202	13)	(203	4)
(210	3)	(213	10)	(214	3)	(215	11)	(216	3)
(223	5)	(227	13)	(228	3)	(229	6)	(230	3)
(241	13)	(242	3)	(243	11)	(244	3)	(255	7)
(257	17)	(258	4)	(269	3)	(271	7)	(283	3)
(285	3)	(297	15)	(298	6)	(299	6)	(313	15)
(314	5)	(340	19)	(341	216)	(342	68)	(343	17)
(355	3)	(356	37)	(357	12)	(358	3)		

NAME:12C_2328.1_1313EC75_Glucose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:233002-10-1

RI:2328

RT:14.440

NUM PEAKS: 123

(70	4)	(72	17)	(73	1000)	(74	88)	(75	83)
(76	4)	(77	10)	(82	7)	(86	6)	(87	6)
(88	3)	(89	34)	(90	3)	(99	5)	(100	12)
(101	38)	(102	11)	(104	4)	(105	24)	(106	4)
(107	3)	(113	6)	(114	10)	(115	12)	(116	16)
(119	7)	(121	3)	(127	4)	(129	69)	(130	17)
(131	27)	(132	4)	(133	65)	(134	9)	(135	16)
(137	6)	(138	3)	(141	3)	(142	5)	(143	11)
(145	7)	(147	141)	(148	22)	(149	18)	(150	3)
(151	7)	(156	3)	(157	35)	(158	9)	(159	4)
(160	94)	(161	19)	(162	4)	(163	6)	(169	4)
(173	4)	(181	8)	(189	11)	(190	3)	(191	16)
(193	10)	(195	8)	(196	3)	(197	3)	(204	17)
(205	7)	(207	16)	(208	4)	(209	3)	(210	4)
(211	43)	(212	9)	(213	5)	(215	4)	(216	6)
(217	36)	(218	9)	(219	4)	(221	3)	(225	13)
(226	3)	(227	9)	(228	6)	(229	5)	(231	7)
(243	5)	(244	3)	(246	3)	(253	4)	(268	3)

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(269	5)	(274	3)	(283	4)	(285	5)	(298	10)
(299	104)	(300	30)	(301	14)	(302	3)	(313	3)
(314	7)	(315	41)	(316	12)	(317	6)	(331	13)
(332	4)	(341	6)	(342	3)	(356	6)	(357	37)
(358	12)	(359	6)	(373	3)	(385	3)	(386	30)
(387	122)	(388	47)	(389	25)	(390	7)	(470	4)
(471	12)	(472	6)	(473	3)				

NAME:12C_2383.7_1313EC75_[724; Glycerol (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:238002-10-1

RI:2384

RT:14.735

NUM PEAKS: 34

(72	16)	(73	1000)	(74	80)	(75	108)	(87	7)
(89	36)	(103	153)	(104	11)	(116	8)	(117	196)
(118	17)	(129	29)	(130	9)	(131	17)	(133	41)
(142	35)	(143	11)	(144	15)	(147	208)	(148	30)
(149	21)	(158	89)	(159	23)	(160	19)	(171	7)
(173	9)	(183	15)	(189	13)	(201	8)	(205	34)
(216	8)	(217	71)	(218	18)	(276	12)		

NAME:12C_2564.4_1313EC75_[945; Galactofuranose-6-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:256001-10-1

RI:2564

RT:15.695

NUM PEAKS: 263

(72	20)	(73	1000)	(74	85)	(75	90)	(76	14)
(77	12)	(79	12)	(84	17)	(86	5)	(87	6)
(88	8)	(89	47)	(90	6)	(91	7)	(92	3)
(96	5)	(98	3)	(100	9)	(101	31)	(103	102)
(105	16)	(106	9)	(107	6)	(115	12)	(116	18)
(117	28)	(119	11)	(120	5)	(121	7)	(128	7)
(129	76)	(130	17)	(131	34)	(132	8)	(133	80)
(134	15)	(135	19)	(136	3)	(137	10)	(139	3)
(142	10)	(143	10)	(144	9)	(145	9)	(146	6)
(147	160)	(148	24)	(151	5)	(153	5)	(156	8)
(157	35)	(158	10)	(159	8)	(162	7)	(163	12)
(165	3)	(166	3)	(171	4)	(172	13)	(173	17)
(174	8)	(175	8)	(176	4)	(181	9)	(185	5)
(186	6)	(188	7)	(189	14)	(190	5)	(191	17)
(195	8)	(196	6)	(197	3)	(200	7)	(201	7)
(202	8)	(203	10)	(204	16)	(205	14)	(206	6)
(207	15)	(208	6)	(210	5)	(211	34)	(212	5)
(214	7)	(216	7)	(217	50)	(218	14)	(219	4)
(220	6)	(222	5)	(223	3)	(225	15)	(226	8)
(227	10)	(228	7)	(229	5)	(230	5)	(231	6)
(232	6)	(233	6)	(235	6)	(236	4)	(239	3)
(240	4)	(241	4)	(245	5)	(249	7)	(250	4)
(251	6)	(253	4)	(259	6)	(260	5)	(264	4)
(265	6)	(266	4)	(267	8)	(268	4)	(269	9)
(270	7)	(271	4)	(273	6)	(274	6)	(275	5)
(276	6)	(281	5)	(282	5)	(283	10)	(284	8)
(285	8)	(291	3)	(292	5)	(293	4)	(295	3)
(296	5)	(298	10)	(299	92)	(300	25)	(301	17)
(302	4)	(303	3)	(305	7)	(306	5)	(307	8)
(308	4)	(312	3)	(313	7)	(314	5)	(315	38)
(316	15)	(317	9)	(318	5)	(319	5)	(320	4)
(321	6)	(324	4)	(326	4)	(327	5)	(328	5)

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(331	12)	(332	9)	(333	7)	(340	5)	(341	8)
(344	3)	(346	3)	(348	4)	(349	6)	(350	7)
(353	5)	(354	3)	(355	6)	(356	10)	(357	35)
(358	14)	(359	8)	(362	5)	(363	4)	(364	3)
(365	4)	(369	6)	(370	6)	(371	7)	(372	6)
(373	6)	(377	4)	(382	3)	(384	4)	(385	7)
(386	28)	(387	115)	(388	44)	(389	28)	(390	9)
(391	5)	(393	3)	(396	5)	(400	4)	(403	6)
(404	3)	(405	6)	(408	5)	(409	4)	(413	3)
(417	7)	(418	6)	(423	5)	(427	4)	(428	3)
(442	6)	(443	3)	(444	3)	(448	7)	(449	4)
(452	3)	(457	6)	(458	8)	(459	3)	(461	5)
(471	17)	(472	7)	(473	6)	(475	3)	(483	6)
(484	3)	(485	3)	(486	5)	(487	6)	(488	4)
(490	4)	(491	4)	(492	4)	(495	7)	(496	5)
(499	3)	(500	4)	(502	3)	(509	5)	(513	7)
(514	3)	(517	6)	(520	6)	(525	4)	(526	4)
(527	5)	(528	4)	(530	7)	(531	6)	(533	3)
(538	5)	(541	3)	(545	3)	(547	4)	(548	3)
(549	3)	(550	3)	(554	4)	(560	4)	(561	4)
(564	4)	(566	4)	(572	4)				

NAME:12C_2619.2_1313EC75_[892; Sucrose (8TMS); alpha-D-Glc-(1,2)-beta-D-Fru]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:262001-10-1

RI:2619

RT:15.985

NUM PEAKS: 126

(70	4)	(71	6)	(72	15)	(73	1000)	(74	87)
(75	134)	(76	8)	(77	10)	(81	25)	(83	5)
(85	9)	(87	7)	(88	3)	(89	17)	(91	3)
(95	3)	(97	7)	(99	9)	(101	27)	(102	5)
(103	193)	(104	18)	(105	11)	(109	13)	(111	10)
(113	10)	(115	9)	(116	18)	(117	78)	(118	8)
(119	8)	(127	7)	(129	177)	(130	22)	(131	39)
(132	10)	(133	53)	(134	7)	(135	6)	(139	4)
(141	6)	(142	6)	(143	28)	(144	5)	(145	18)
(146	3)	(147	214)	(148	34)	(149	36)	(150	5)
(151	4)	(153	7)	(155	46)	(156	8)	(157	37)
(158	6)	(159	9)	(161	3)	(163	6)	(169	89)
(170	15)	(171	18)	(172	3)	(173	14)	(175	5)
(177	6)	(183	19)	(184	3)	(185	3)	(189	33)
(190	8)	(191	123)	(192	22)	(193	11)	(199	25)
(200	4)	(201	4)	(203	13)	(204	57)	(205	23)
(206	7)	(207	5)	(215	6)	(216	5)	(217	307)
(218	74)	(219	39)	(220	6)	(221	9)	(227	3)
(229	6)	(230	6)	(231	15)	(232	5)	(233	7)
(234	3)	(241	3)	(242	4)	(243	40)	(244	11)
(245	13)	(246	3)	(247	6)	(257	5)	(259	20)
(260	6)	(263	6)	(271	27)	(272	7)	(273	11)
(274	3)	(289	25)	(290	7)	(291	7)	(305	5)
(319	9)	(320	4)	(331	20)	(332	16)	(333	7)
(360	13)	(361	126)	(362	45)	(363	21)	(364	5)
(377	4)								

NAME:12C_2656.9_1313EC75_[559; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:266001-10-1

RI:2657

185

RT:16.186

NUM PEAKS: 42

(70	175)	(72	21)	(73	1000)	(74	83)	(75	109)
(80	19)	(81	16)	(82	45)	(83	15)	(89	44)
(98	52)	(99	122)	(100	21)	(103	162)	(113	15)
(116	16)	(117	56)	(125	36)	(127	130)	(128	21)
(129	58)	(131	29)	(133	55)	(147	201)	(148	37)
(149	29)	(155	15)	(156	16)	(169	37)	(170	18)
(171	44)	(185	29)	(189	14)	(196	25)	(217	97)
(218	25)	(238	14)	(267	27)	(268	44)	(292	50)
(298	48)	(323	21)						

NAME:12C_2733.0_1313EC75_[840; Maltose methoxyamine (8TMS); alpha-D-Glc-(1,4)-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:273002-10-1

RI:2733

RT:16.590

NUM PEAKS: 78

(70	3)	(72	11)	(73	1000)	(74	85)	(82	17)
(83	4)	(85	5)	(86	5)	(87	4)	(88	4)
(89	48)	(90	3)	(100	7)	(101	19)	(102	5)
(103	113)	(104	9)	(105	32)	(106	3)	(113	5)
(114	6)	(115	5)	(116	8)	(117	77)	(118	9)
(119	5)	(128	4)	(130	10)	(131	14)	(132	3)
(133	44)	(140	3)	(141	4)	(143	15)	(147	303)
(148	48)	(149	26)	(156	4)	(160	85)	(161	20)
(162	5)	(163	5)	(169	37)	(170	7)	(175	3)
(186	10)	(187	3)	(189	23)	(190	3)	(203	6)
(204	267)	(205	112)	(206	33)	(207	11)	(215	4)
(216	6)	(218	17)	(221	5)	(222	3)	(229	7)
(230	3)	(243	19)	(244	35)	(245	12)	(269	5)
(270	3)	(271	18)	(272	4)	(307	6)	(318	4)
(319	23)	(320	9)	(360	20)	(361	169)	(362	60)
(363	26)	(390	3)	(451	4)				

NAME:12C_2826.4_1313EC75_[855; Squalene]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:283001-10-1

RI:2826

RT:17.062

NUM PEAKS: 34

(70	112)	(79	130)	(80	53)	(81	1000)	(82	107)
(87	13)	(92	36)	(93	202)	(95	280)	(97	45)
(107	124)	(108	40)	(109	123)	(118	14)	(120	20)
(121	171)	(122	37)	(123	102)	(132	9)	(135	89)
(136	134)	(137	123)	(138	11)	(149	107)	(158	24)
(163	31)	(173	24)	(174	16)	(175	26)	(203	30)
(231	33)	(259	18)	(260	15)	(363	10)		

NAME:12C_2871.8_1313EC75_Isomaltose methoxyamine (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:287001-10-1

RI:2872

RT:17.263

NUM PEAKS: 126

(70	5)	(71	5)	(72	15)	(73	1000)	(74	87)
(75	96)	(81	15)	(82	4)	(83	4)	(85	8)
(86	4)	(87	7)	(88	3)	(89	33)	(90	3)

186

(97 5) (99 8) (100 17) (101 36) (102 12)
 (103 125) (104 12) (105 24) (109 7) (111 6)
 (113 7) (114 6) (115 9) (116 20) (117 72)
 (118 7) (119 6) (127 5) (128 4) (129 122)
 (130 20) (131 30) (132 6) (133 56) (134 7)
 (135 5) (139 3) (141 5) (142 7) (143 23)
 (144 4) (145 9) (147 236) (148 37) (149 28)
 (150 3) (151 3) (153 4) (155 18) (156 4)
 (158 6) (159 5) (160 95) (161 39) (162 7)
 (163 9) (169 67) (170 11) (171 8) (172 3)
 (173 6) (174 3) (175 4) (177 4) (183 5)
 (189 32) (190 9) (191 52) (192 9) (193 4)
 (201 3) (203 14) (204 215) (205 57) (206 20)
 (207 7) (215 5) (216 7) (217 135) (218 34)
 (219 15) (221 9) (228 5) (229 7) (230 5)
 (231 16) (232 5) (233 8) (234 3) (241 3)
 (243 31) (244 10) (245 8) (246 5) (247 5)
 (257 3) (259 6) (262 3) (271 24) (272 6)
 (273 6) (274 4) (275 3) (291 7) (300 3)
 (305 8) (306 4) (307 5) (317 3) (318 3)
 (319 15) (320 5) (331 6) (332 5) (360 18)
 (361 158) (362 56) (363 25) (364 9) (390 4)
 (480 4)

NAME:12C_2906.7_1313EC75_Isomaltose methoxyamine (BP) (8TMS); alpha-D-Glc-(1,6)-D-Glc (8TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:291002-10-1

RI:2907

RT:17.418

NUM PEAKS: 64

(72 14) (73 1000) (74 80) (75 86) (81 13)
 (87 7) (89 41) (100 18) (101 36) (102 11)
 (103 166) (104 15) (105 15) (115 7) (117 69)
 (118 8) (129 110) (130 17) (131 29) (132 6)
 (133 73) (134 9) (143 20) (147 235) (148 37)
 (149 28) (155 17) (157 19) (160 77) (161 41)
 (163 9) (169 65) (170 11) (171 6) (173 6)
 (189 29) (190 8) (191 51) (192 8) (201 5)
 (203 15) (204 212) (205 60) (206 19) (216 4)
 (217 106) (218 29) (219 13) (221 6) (229 7)
 (233 16) (243 29) (244 9) (271 22) (273 12)
 (274 4) (305 9) (319 14) (331 6) (332 4)
 (360 19) (361 152) (362 56) (363 27)

NAME:12C_2811.2_1160EC39_[895; Isomaltose methoxyamine (8TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:281001-10-1

RI:2811

RT:17.476

NUM PEAKS: 89

(73 1000) (74 66) (75 95) (89 31) (101 47)
 (103 92) (104 28) (105 26) (109 8) (116 13)
 (117 75) (118 9) (129 104) (131 19) (133 36)
 (134 8) (143 19) (147 179) (148 39) (150 9)
 (157 13) (160 85) (161 45) (164 17) (169 21)
 (171 10) (174 10) (189 24) (191 47) (203 10)
 (204 304) (205 63) (206 37) (214 12) (217 102)
 (218 34) (219 11) (228 18) (230 12) (240 14)
 (243 30) (244 8) (245 5) (248 13) (259 11)

187

(262	9)	(271	35)	(273	13)	(276	11)	(287	9)
(304	6)	(319	14)	(322	10)	(325	6)	(342	9)
(344	7)	(346	8)	(352	12)	(361	87)	(362	45)
(363	21)	(365	12)	(367	8)	(375	12)	(395	14)
(396	7)	(399	9)	(405	5)	(407	7)	(420	7)
(421	5)	(433	12)	(436	6)	(439	10)	(463	11)
(464	16)	(468	7)	(475	11)	(480	10)	(482	6)
(486	7)	(493	7)	(497	16)	(506	11)	(527	7)
(529	18)	(562	11)	(564	5)	(581	3)		

NAME:12C_2518.0_1313EC75_[644; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:252002-10-1

RI:2518

RT:15.448

NUM PEAKS: 176

(70	13)	(71	26)	(72	19)	(73	1000)	(74	84)
(75	108)	(76	5)	(77	6)	(78	3)	(79	4)
(80	8)	(81	8)	(82	13)	(83	15)	(84	14)
(85	22)	(86	8)	(87	6)	(88	3)	(89	43)
(90	4)	(91	3)	(93	3)	(94	4)	(95	9)
(96	52)	(97	23)	(98	28)	(99	11)	(100	7)
(101	15)	(102	7)	(103	197)	(104	19)	(105	13)
(106	4)	(107	9)	(108	4)	(110	4)	(111	7)
(112	6)	(113	13)	(114	8)	(115	6)	(116	7)
(117	58)	(118	6)	(119	7)	(122	5)	(123	11)
(124	3)	(125	4)	(126	6)	(127	6)	(128	16)
(129	42)	(130	6)	(131	19)	(132	3)	(133	52)
(134	7)	(135	11)	(136	6)	(138	3)	(139	3)
(140	7)	(141	7)	(142	24)	(143	13)	(144	6)
(145	4)	(147	207)	(148	32)	(149	21)	(150	5)
(151	3)	(152	4)	(153	3)	(154	6)	(155	7)
(156	99)	(157	23)	(158	11)	(159	3)	(160	5)
(161	3)	(163	6)	(166	3)	(167	5)	(168	7)
(169	4)	(170	21)	(171	4)	(172	6)	(173	36)
(174	4)	(175	4)	(177	3)	(179	3)	(180	3)
(181	6)	(182	4)	(183	5)	(184	3)	(185	3)
(186	61)	(187	11)	(188	4)	(189	19)	(190	5)
(191	8)	(192	3)	(195	3)	(196	3)	(197	4)
(198	6)	(202	4)	(203	3)	(204	13)	(205	27)
(206	6)	(207	6)	(209	4)	(213	5)	(214	51)
(215	8)	(216	5)	(217	68)	(218	14)	(219	6)
(221	5)	(224	3)	(225	13)	(226	4)	(229	3)
(230	6)	(237	6)	(244	7)	(246	4)	(253	3)
(255	3)	(258	3)	(269	3)	(270	3)	(274	6)
(275	3)	(277	3)	(287	3)	(291	3)	(299	6)
(300	3)	(307	6)	(313	7)	(319	3)	(327	4)
(343	14)	(344	6)	(345	4)	(346	10)	(347	4)
(355	4)	(356	3)	(372	3)	(373	10)	(374	11)
(375	5)	(411	3)	(414	3)	(415	15)	(416	11)
(417	9)	(444	3)	(445	16)	(446	65)	(447	28)
(448	11)								

NAME:12C_2493.1_1313EC75_[657; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:249001-10-1

RI:2493

RT:15.316

NUM PEAKS: 236

(72	14)	(73	1000)	(74	83)	(75	95)	(76	9)
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188

(77	5)	(80	5)	(82	4)	(84	6)	(86	3)
(87	14)	(88	4)	(89	37)	(90	4)	(93	5)
(94	4)	(95	7)	(96	35)	(97	6)	(98	18)
(100	8)	(101	16)	(102	8)	(103	188)	(104	15)
(105	12)	(106	3)	(107	10)	(108	5)	(114	8)
(115	4)	(116	4)	(117	51)	(118	6)	(119	9)
(122	3)	(123	9)	(124	3)	(126	3)	(128	14)
(129	39)	(130	7)	(131	17)	(133	43)	(134	6)
(135	10)	(137	3)	(138	3)	(139	3)	(140	6)
(142	23)	(143	12)	(144	5)	(145	4)	(146	4)
(147	218)	(148	35)	(149	22)	(150	5)	(151	3)
(152	5)	(154	6)	(156	74)	(157	20)	(158	8)
(159	3)	(160	5)	(161	4)	(162	3)	(163	5)
(164	4)	(166	4)	(167	6)	(168	6)	(170	22)
(171	4)	(172	6)	(173	39)	(174	9)	(175	8)
(176	4)	(177	3)	(179	5)	(180	5)	(181	5)
(182	4)	(184	3)	(186	30)	(187	8)	(188	6)
(189	17)	(190	6)	(191	10)	(192	3)	(193	4)
(195	5)	(196	7)	(198	8)	(199	4)	(200	5)
(202	4)	(203	3)	(204	6)	(205	27)	(206	6)
(207	10)	(209	5)	(214	23)	(215	4)	(216	3)
(217	70)	(218	15)	(219	5)	(220	3)	(221	14)
(222	3)	(223	5)	(224	4)	(225	11)	(226	3)
(227	4)	(229	3)	(230	4)	(231	4)	(235	3)
(236	4)	(237	5)	(239	3)	(240	3)	(241	3)
(244	5)	(246	3)	(247	4)	(249	4)	(250	4)
(251	4)	(252	3)	(253	5)	(254	3)	(255	4)
(256	5)	(258	5)	(263	3)	(265	4)	(266	5)
(268	4)	(269	4)	(270	5)	(271	3)	(273	3)
(274	9)	(275	5)	(276	3)	(277	6)	(278	4)
(279	3)	(281	6)	(283	3)	(284	3)	(286	4)
(288	4)	(295	4)	(307	10)	(311	3)	(313	9)
(314	4)	(316	3)	(319	3)	(320	4)	(326	3)
(327	5)	(328	3)	(329	4)	(330	3)	(331	3)
(332	3)	(338	4)	(339	3)	(340	3)	(342	3)
(343	13)	(344	8)	(345	4)	(346	10)	(347	6)
(348	3)	(349	3)	(351	3)	(355	5)	(356	4)
(362	3)	(367	3)	(372	3)	(373	18)	(374	14)
(375	6)	(376	4)	(378	3)	(380	3)	(391	3)
(395	3)	(398	3)	(406	3)	(411	3)	(412	3)
(414	5)	(415	17)	(416	12)	(417	7)	(418	4)
(423	3)	(429	3)	(430	3)	(431	4)	(437	4)
(438	3)	(442	3)	(443	4)	(444	3)	(445	20)
(446	69)	(447	32)	(448	13)	(449	5)	(457	3)
(461	3)	(462	3)	(468	3)	(469	4)	(486	3)
(515	3)	(522	4)	(534	3)	(539	3)	(540	3)
(543	3)								

NAME:12C_2134.7_1274EC17_[904; Galactose methoxyamine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:214003-10-1

RI:2135

RT:13.842

NUM PEAKS: 108

(70	5)	(72	15)	(73	1000)	(74	79)	(75	66)
(83	16)	(84	20)	(87	5)	(89	48)	(90	6)
(92	3)	(100	12)	(101	13)	(102	5)	(103	217)
(104	20)	(105	11)	(112	3)	(113	7)	(114	10)
(115	6)	(116	4)	(117	82)	(118	8)	(119	8)
(120	3)	(127	4)	(129	97)	(130	15)	(131	24)

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(133	98)	(134	12)	(135	8)	(138	3)	(141	4)
(142	5)	(143	12)	(147	261)	(148	40)	(149	23)
(150	3)	(155	4)	(156	3)	(157	111)	(158	15)
(159	10)	(163	10)	(166	4)	(171	3)	(172	29)
(173	18)	(174	5)	(175	6)	(177	5)	(189	29)
(190	11)	(191	17)	(193	4)	(200	3)	(201	9)
(202	5)	(203	5)	(204	27)	(205	168)	(206	32)
(207	16)	(214	3)	(216	5)	(217	112)	(218	23)
(219	9)	(227	3)	(229	27)	(230	11)	(231	8)
(232	3)	(233	4)	(235	4)	(243	3)	(244	3)
(245	4)	(247	3)	(257	3)	(260	3)	(262	8)
(263	7)	(268	5)	(271	4)	(272	4)	(273	4)
(274	4)	(277	5)	(288	4)	(291	7)	(302	4)
(305	7)	(306	5)	(307	8)	(318	3)	(319	217)
(320	68)	(321	33)	(322	6)	(332	6)	(333	3)
(378	3)	(402	4)	(514	4)				

NAME:12C_2128.7_1274EC17_[857; Mannitol (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:213001-10-1

RI:2129

RT:13.804

NUM PEAKS: 237

(70	18)	(71	81)	(72	20)	(73	1000)	(74	82)
(75	77)	(76	6)	(77	5)	(79	3)	(80	6)
(81	13)	(82	15)	(83	59)	(84	48)	(85	60)
(86	9)	(87	6)	(88	6)	(89	52)	(90	5)
(92	3)	(93	19)	(94	6)	(95	12)	(96	4)
(97	41)	(98	8)	(99	28)	(100	7)	(101	15)
(102	5)	(103	200)	(104	21)	(105	21)	(106	5)
(110	4)	(111	25)	(112	9)	(113	21)	(114	28)
(115	9)	(116	5)	(117	71)	(118	7)	(119	12)
(120	3)	(121	3)	(123	11)	(125	16)	(126	6)
(127	17)	(128	5)	(129	103)	(130	24)	(131	25)
(133	66)	(134	10)	(135	10)	(138	4)	(139	5)
(140	5)	(141	10)	(142	9)	(143	16)	(144	5)
(146	12)	(147	261)	(148	39)	(149	29)	(150	4)
(151	4)	(152	4)	(153	5)	(154	5)	(155	10)
(156	4)	(157	112)	(158	17)	(159	6)	(160	3)
(161	4)	(162	4)	(163	14)	(164	3)	(165	3)
(167	3)	(168	5)	(169	6)	(170	6)	(171	3)
(172	8)	(173	13)	(175	5)	(176	3)	(177	5)
(180	4)	(181	5)	(182	4)	(183	3)	(184	5)
(185	4)	(186	3)	(187	3)	(188	5)	(189	29)
(190	10)	(191	21)	(192	6)	(198	6)	(200	3)
(201	5)	(202	8)	(203	7)	(204	31)	(205	167)
(206	33)	(207	14)	(210	3)	(211	4)	(214	4)
(215	6)	(216	7)	(217	116)	(218	24)	(219	11)
(220	6)	(224	3)	(228	3)	(229	26)	(230	12)
(231	9)	(232	4)	(233	4)	(238	4)	(240	4)
(242	4)	(243	5)	(244	4)	(245	3)	(246	4)
(247	3)	(248	3)	(254	4)	(255	3)	(256	3)
(257	4)	(262	34)	(263	13)	(264	5)	(266	4)
(270	3)	(271	3)	(275	3)	(277	7)	(278	6)
(280	4)	(284	3)	(288	5)	(289	3)	(290	4)
(291	9)	(292	4)	(304	4)	(305	6)	(306	3)
(307	8)	(308	5)	(309	3)	(311	3)	(312	4)
(313	3)	(318	6)	(319	227)	(320	73)	(321	31)
(322	7)	(323	4)	(330	3)	(331	5)	(332	3)
(333	4)	(334	6)	(335	4)	(336	6)	(337	4)

190

(338	3)	(339	4)	(340	3)	(342	3)	(344	3)
(345	3)	(347	3)	(352	4)	(358	3)	(364	4)
(368	3)	(374	4)	(376	4)	(377	3)	(380	4)
(381	3)	(386	3)	(390	3)	(391	3)	(392	3)
(393	3)	(400	3)	(401	4)	(402	5)	(404	3)
(405	3)	(407	3)	(419	3)	(436	3)	(437	3)
(446	4)	(457	3)	(459	3)	(464	3)	(466	4)
(467	3)	(476	3)	(484	3)	(485	3)	(486	3)
(488	3)	(489	3)	(500	3)	(504	3)	(508	3)
(512	3)	(513	3)	(515	3)	(516	3)	(518	3)
(528	4)	(548	3)						

NAME:12C 2217.8_1274EC17_9-(Z)-Octadecenoic acid (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:222001-10-1

RI:2218

RT:14.350

NUM PEAKS: 146

(70	43)	(71	11)	(72	39)	(73	838)	(74	88)
(75	1000)	(76	67)	(77	66)	(78	11)	(79	84)
(80	36)	(81	189)	(82	96)	(83	144)	(84	190)
(85	26)	(86	9)	(87	7)	(88	6)	(89	27)
(90	3)	(91	28)	(92	9)	(93	49)	(94	34)
(95	140)	(96	230)	(97	128)	(98	156)	(99	29)
(101	10)	(102	3)	(103	3)	(105	30)	(106	8)
(107	27)	(108	22)	(109	75)	(110	86)	(111	58)
(112	31)	(113	5)	(116	27)	(117	731)	(118	73)
(119	53)	(120	8)	(121	34)	(122	11)	(123	57)
(124	37)	(125	21)	(126	6)	(128	5)	(129	552)
(130	70)	(131	105)	(132	135)	(133	56)	(134	27)
(135	17)	(136	6)	(137	41)	(138	31)	(139	11)
(140	4)	(141	3)	(142	4)	(143	38)	(144	7)
(145	243)	(146	33)	(147	35)	(148	16)	(149	13)
(150	5)	(151	26)	(152	41)	(153	7)	(155	26)
(156	7)	(157	16)	(158	8)	(159	20)	(160	3)
(161	7)	(162	4)	(163	4)	(164	4)	(165	14)
(166	23)	(167	8)	(168	3)	(169	16)	(170	9)
(171	26)	(172	10)	(173	11)	(174	5)	(175	4)
(179	6)	(180	34)	(181	6)	(183	21)	(184	6)
(185	59)	(186	14)	(187	11)	(188	5)	(193	4)
(194	5)	(199	80)	(200	14)	(201	13)	(206	3)
(207	8)	(208	3)	(213	11)	(214	3)	(217	14)
(218	7)	(220	10)	(221	10)	(222	44)	(223	9)
(227	4)	(235	5)	(236	7)	(241	8)	(246	4)
(255	3)	(257	5)	(258	3)	(264	34)	(265	8)
(272	4)	(294	4)	(295	9)	(296	3)	(311	3)
(338	3)	(339	112)	(340	40)	(341	9)	(354	14)
(355	5)								

NAME:12C 2278.6_1274EC17_[583; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:228001-10-1

RI:2279

RT:14.672

NUM PEAKS: 235

(70	4)	(71	45)	(72	28)	(73	1000)	(74	86)
(75	49)	(77	27)	(78	15)	(79	33)	(80	21)
(81	24)	(85	15)	(87	9)	(89	27)	(91	32)
(92	21)	(93	66)	(94	12)	(98	5)	(100	9)
(101	6)	(102	3)	(103	77)	(105	24)	(113	5)

191

(114	8)	(117	74)	(122	9)	(126	10)	(128	10)
(129	20)	(131	17)	(133	131)	(134	61)	(137	3)
(139	6)	(140	7)	(142	9)	(143	6)	(144	5)
(145	4)	(147	194)	(148	40)	(149	18)	(150	9)
(151	9)	(152	9)	(153	6)	(154	3)	(157	16)
(158	5)	(159	8)	(163	6)	(164	3)	(165	7)
(168	7)	(170	5)	(172	12)	(173	12)	(176	3)
(180	4)	(183	12)	(186	13)	(188	5)	(189	21)
(190	19)	(191	12)	(194	7)	(197	4)	(199	11)
(201	34)	(202	15)	(204	13)	(205	45)	(206	11)
(212	8)	(213	3)	(214	21)	(215	7)	(216	8)
(217	58)	(218	19)	(219	4)	(222	3)	(224	5)
(226	15)	(227	7)	(229	9)	(230	4)	(231	6)
(233	7)	(234	15)	(235	8)	(236	4)	(241	6)
(243	4)	(244	9)	(245	7)	(246	24)	(247	8)
(248	6)	(251	3)	(252	6)	(254	13)	(256	5)
(257	4)	(258	4)	(260	11)	(265	5)	(266	7)
(267	4)	(268	12)	(269	11)	(270	5)	(274	3)
(275	9)	(278	7)	(282	4)	(284	10)	(285	4)
(286	9)	(287	4)	(288	3)	(289	8)	(290	149)
(291	42)	(292	18)	(293	10)	(294	11)	(295	3)
(296	6)	(301	5)	(306	3)	(307	4)	(308	5)
(310	5)	(315	5)	(316	6)	(317	5)	(319	36)
(320	15)	(325	6)	(327	4)	(331	8)	(335	3)
(336	5)	(346	5)	(347	9)	(348	5)	(352	5)
(354	6)	(355	7)	(356	4)	(359	4)	(360	5)
(361	3)	(364	6)	(365	8)	(367	8)	(368	4)
(369	4)	(374	4)	(380	6)	(381	3)	(382	3)
(383	5)	(384	5)	(385	6)	(387	12)	(388	10)
(389	3)	(390	5)	(392	3)	(393	3)	(394	3)
(395	3)	(404	8)	(405	6)	(406	3)	(409	5)
(410	4)	(411	3)	(412	7)	(413	5)	(414	4)
(416	7)	(421	7)	(422	3)	(424	9)	(425	9)
(428	3)	(430	8)	(431	5)	(433	6)	(434	3)
(437	3)	(440	5)	(445	4)	(448	4)	(452	5)
(453	5)	(462	4)	(465	6)	(468	5)	(473	4)
(476	4)	(477	4)	(481	5)	(483	3)	(486	6)
(489	10)	(492	5)	(494	3)	(498	4)	(499	5)
(504	5)	(513	4)	(521	8)	(522	10)	(524	3)
(525	10)	(530	4)	(535	3)	(538	7)	(539	4)
(541	8)	(542	4)	(543	3)	(545	3)	(549	6)
(550	3)	(556	6)	(567	3)	(571	3)	(590	3)

NAME:12C_2294.6_1274EC17_[877; beta-D-Galactopyranoside-(1,2)-glycerol
(6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:230001-10-1

RI:2295

RT:14.757

NUM PEAKS: 71

(73	1000)	(74	70)	(75	80)	(78	15)	(87	12)
(89	11)	(101	47)	(103	223)	(104	21)	(116	10)
(117	53)	(118	11)	(129	115)	(130	32)	(131	42)
(133	29)	(134	15)	(135	15)	(143	10)	(147	207)
(148	42)	(149	19)	(154	17)	(161	9)	(163	8)
(189	29)	(191	72)	(192	19)	(202	10)	(203	32)
(204	676)	(205	142)	(206	48)	(217	119)	(218	42)
(219	50)	(223	7)	(231	21)	(232	10)	(240	8)
(242	8)	(243	17)	(258	6)	(274	15)	(280	6)
(281	15)	(286	8)	(293	10)	(295	8)	(296	13)

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(297	9)	(298	9)	(303	12)	(319	14)	(324	9)
(331	12)	(337	70)	(338	25)	(359	8)	(382	7)
(383	7)	(414	10)	(450	11)	(464	7)	(489	18)
(493	16)	(494	9)	(511	9)	(512	13)	(574	4)
(579	4)								

NAME:12C_2311.4_1274EC17_Galactose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232001-10-1

RI:2311

RT:14.846

NUM PEAKS: 321

(70	43)	(71	90)	(72	74)	(73	1000)	(74	112)
(75	212)	(76	6)	(82	7)	(84	27)	(86	15)
(87	21)	(88	19)	(89	37)	(90	8)	(96	14)
(98	9)	(100	24)	(101	135)	(102	17)	(110	10)
(112	21)	(113	6)	(114	19)	(116	13)	(124	14)
(129	12)	(130	45)	(140	6)	(144	17)	(147	237)
(148	22)	(149	11)	(150	14)	(157	46)	(158	27)
(160	159)	(162	6)	(163	11)	(166	3)	(168	7)
(169	12)	(174	8)	(175	8)	(177	10)	(178	11)
(179	16)	(181	13)	(182	20)	(183	4)	(184	6)
(189	5)	(191	27)	(192	14)	(193	13)	(195	13)
(196	19)	(197	6)	(203	4)	(204	18)	(205	18)
(206	21)	(207	35)	(208	7)	(209	13)	(210	5)
(211	39)	(212	17)	(216	17)	(217	23)	(218	10)
(220	21)	(221	23)	(222	21)	(223	10)	(224	8)
(225	8)	(228	13)	(229	14)	(230	8)	(231	21)
(232	10)	(233	15)	(234	15)	(235	8)	(238	2)
(242	5)	(245	5)	(246	10)	(247	19)	(248	3)
(249	9)	(250	15)	(251	18)	(252	9)	(253	17)
(254	14)	(255	12)	(256	5)	(257	10)	(258	3)
(261	9)	(262	9)	(263	15)	(264	11)	(265	15)
(266	4)	(267	9)	(270	4)	(271	5)	(272	8)
(273	3)	(274	9)	(277	12)	(278	4)	(279	9)
(280	8)	(281	14)	(282	10)	(283	8)	(284	7)
(285	17)	(286	9)	(287	9)	(289	6)	(290	5)
(291	10)	(292	7)	(293	3)	(294	6)	(295	13)
(297	5)	(298	6)	(299	130)	(300	36)	(301	21)
(302	17)	(303	18)	(304	7)	(305	9)	(306	7)
(307	8)	(308	12)	(309	2)	(313	6)	(314	6)
(316	5)	(319	9)	(323	9)	(324	7)	(325	10)
(326	5)	(328	161)	(329	79)	(330	10)	(331	29)
(332	3)	(336	6)	(337	13)	(339	8)	(340	5)
(341	10)	(342	8)	(343	8)	(345	4)	(347	2)
(352	11)	(353	6)	(354	15)	(355	11)	(356	4)
(357	51)	(358	21)	(359	21)	(360	6)	(362	2)
(363	3)	(364	8)	(365	5)	(368	8)	(369	6)
(370	7)	(371	18)	(373	5)	(374	12)	(377	10)
(378	4)	(379	13)	(380	11)	(382	12)	(386	23)
(387	220)	(388	103)	(389	47)	(390	7)	(392	11)
(394	10)	(395	11)	(396	10)	(397	14)	(398	8)
(399	3)	(402	7)	(403	9)	(404	14)	(405	15)
(406	6)	(407	9)	(408	4)	(412	5)	(413	11)
(414	9)	(415	4)	(416	15)	(417	13)	(423	8)
(424	11)	(425	11)	(427	3)	(429	12)	(433	5)
(434	6)	(436	13)	(437	7)	(438	4)	(439	5)
(441	5)	(442	4)	(443	15)	(444	9)	(446	10)
(447	5)	(448	6)	(449	17)	(450	6)	(451	5)
(452	4)	(453	3)	(454	9)	(455	4)	(457	8)

193

(458	11)	(461	10)	(462	5)	(464	5)	(465	8)
(466	9)	(469	13)	(470	3)	(471	21)	(472	25)
(473	20)	(474	6)	(475	3)	(476	12)	(477	5)
(478	10)	(480	5)	(483	2)	(484	13)	(485	11)
(486	5)	(487	4)	(489	6)	(490	10)	(491	9)
(492	4)	(493	6)	(496	14)	(498	4)	(501	10)
(502	6)	(504	18)	(505	6)	(507	22)	(508	10)
(511	8)	(514	4)	(515	12)	(516	3)	(518	6)
(522	6)	(523	5)	(524	2)	(525	7)	(528	2)
(529	12)	(531	2)	(532	8)	(533	2)	(534	4)
(535	4)	(538	2)	(539	4)	(540	6)	(541	2)
(542	5)	(543	16)	(547	5)	(549	2)	(550	4)
(552	5)	(553	3)	(559	2)	(564	2)	(565	2)
(566	5)	(568	11)	(569	5)	(571	2)	(572	1)
(574	2)	(575	5)	(580	3)	(581	1)	(585	2)
(586	2)	(588	4)	(590	1)	(593	3)	(596	2)
(598	1)								

NAME:12C_2474.9_1274EC17_[945; Uridine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:248002-10-1

RI:2475

RT:15.711

NUM PEAKS: 131

(70	12)	(71	8)	(72	22)	(73	1000)	(74	84)
(75	136)	(76	9)	(77	10)	(79	3)	(81	8)
(82	6)	(83	4)	(84	4)	(85	13)	(86	4)
(87	7)	(89	16)	(94	3)	(95	5)	(96	8)
(97	14)	(98	5)	(99	49)	(100	14)	(101	28)
(102	7)	(103	175)	(104	16)	(105	9)	(110	3)
(111	9)	(112	4)	(113	19)	(114	4)	(115	39)
(116	11)	(117	29)	(118	3)	(119	8)	(124	4)
(125	5)	(126	10)	(127	10)	(128	4)	(129	74)
(130	10)	(131	26)	(132	4)	(133	68)	(134	9)
(135	8)	(137	3)	(138	5)	(140	6)	(141	7)
(142	7)	(143	33)	(144	5)	(145	8)	(147	171)
(148	47)	(149	36)	(150	5)	(151	3)	(153	15)
(154	6)	(155	6)	(156	4)	(157	13)	(158	3)
(159	5)	(163	7)	(167	3)	(168	11)	(169	154)
(170	23)	(171	15)	(173	3)	(174	3)	(175	3)
(177	4)	(183	12)	(184	3)	(185	32)	(186	5)
(187	3)	(189	17)	(190	4)	(191	46)	(192	7)
(203	8)	(204	10)	(205	4)	(211	12)	(213	28)
(214	4)	(215	17)	(216	5)	(217	420)	(218	102)
(219	45)	(220	6)	(226	6)	(227	5)	(229	5)
(230	24)	(231	21)	(232	5)	(239	3)	(241	5)
(243	52)	(244	11)	(245	21)	(246	4)	(251	3)
(257	7)	(258	5)	(259	91)	(260	20)	(261	8)
(265	15)	(267	8)	(280	3)	(299	16)	(300	5)
(315	9)	(316	3)	(317	4)	(348	3)	(349	3)
(445	5)								

NAME:12C_2687.5_1274EC17_[964; Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:269002-10-1

RI:2688

RT:16.837

NUM PEAKS: 93

(72	12)	(73	1000)	(74	84)	(75	76)	(81	20)
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194

(94	6)	(101	13)	(103	160)	(104	15)	(107	5)
(113	9)	(115	8)	(116	18)	(117	58)	(127	10)
(129	146)	(130	17)	(131	30)	(133	53)	(135	9)
(142	8)	(143	23)	(144	8)	(145	9)	(147	232)
(148	38)	(149	31)	(153	7)	(155	26)	(157	26)
(158	10)	(163	7)	(169	122)	(170	19)	(171	13)
(177	6)	(181	9)	(183	6)	(189	31)	(190	11)
(191	261)	(192	40)	(193	23)	(199	8)	(203	13)
(204	84)	(205	33)	(207	12)	(211	5)	(217	171)
(218	39)	(219	18)	(229	14)	(230	11)	(231	15)
(233	7)	(242	4)	(243	47)	(244	15)	(245	10)
(257	6)	(258	5)	(259	7)	(265	4)	(271	46)
(272	11)	(273	9)	(282	3)	(287	6)	(291	7)
(292	5)	(319	16)	(320	12)	(321	6)	(331	23)
(332	13)	(361	246)	(362	84)	(363	42)	(364	12)
(374	6)	(387	3)	(435	7)	(451	8)	(452	4)
(455	5)	(456	3)	(461	5)	(507	4)	(512	4)
(524	4)	(528	5)	(574	3)				

NAME:12C_2748.2_1274EC17_Trehalose (8TMS); alpha-D-Glc-(1,1)-alpha-D-Glc

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:274002-10-1

RI:2748

RT:17.158

NUM PEAKS: 213

(70	2)	(71	3)	(72	11)	(73	1000)	(74	89)
(75	89)	(76	5)	(77	4)	(79	1)	(80	1)
(81	23)	(82	2)	(83	5)	(84	1)	(85	8)
(86	1)	(87	6)	(88	2)	(89	15)	(90	2)
(91	2)	(94	1)	(95	2)	(97	4)	(98	1)
(99	7)	(100	1)	(101	20)	(102	5)	(103	243)
(104	23)	(105	11)	(109	12)	(110	1)	(111	5)
(112	1)	(113	13)	(114	4)	(115	9)	(116	12)
(117	67)	(118	7)	(119	8)	(120	1)	(125	1)
(126	1)	(127	7)	(128	2)	(129	192)	(130	24)
(131	39)	(132	6)	(133	52)	(134	8)	(135	5)
(139	4)	(140	1)	(141	5)	(142	6)	(143	26)
(144	4)	(145	9)	(146	2)	(147	287)	(148	45)
(149	37)	(150	5)	(151	3)	(153	5)	(154	2)
(155	28)	(156	6)	(157	26)	(158	4)	(159	5)
(160	1)	(161	4)	(162	1)	(163	6)	(164	1)
(165	1)	(167	2)	(168	1)	(169	142)	(170	24)
(171	13)	(172	2)	(173	8)	(174	2)	(175	5)
(176	1)	(177	5)	(178	1)	(179	1)	(181	2)
(182	1)	(183	6)	(184	1)	(185	2)	(187	2)
(189	23)	(190	7)	(191	347)	(192	66)	(193	31)
(194	4)	(195	1)	(199	4)	(200	1)	(201	3)
(202	3)	(203	12)	(204	98)	(205	37)	(206	12)
(207	7)	(208	1)	(215	5)	(216	2)	(217	177)
(218	47)	(219	22)	(220	4)	(221	12)	(222	3)
(223	2)	(227	4)	(228	2)	(229	16)	(230	10)
(231	15)	(232	5)	(233	10)	(234	3)	(235	1)
(239	1)	(241	6)	(242	3)	(243	59)	(244	18)
(245	17)	(246	4)	(247	5)	(248	1)	(249	1)
(255	3)	(256	1)	(257	7)	(258	2)	(259	6)
(260	2)	(261	1)	(263	6)	(264	1)	(265	5)
(266	1)	(267	1)	(270	1)	(271	71)	(272	18)
(273	11)	(274	2)	(275	1)	(277	1)	(278	1)
(279	7)	(280	2)	(281	1)	(287	2)	(288	1)
(289	1)	(290	9)	(291	12)	(292	5)	(293	3)

195

(303	1)	(304	1)	(305	9)	(306	4)	(307	3)
(308	1)	(317	4)	(318	3)	(319	22)	(320	11)
(321	5)	(322	2)	(323	3)	(324	1)	(331	22)
(332	14)	(333	8)	(334	3)	(335	1)	(345	2)
(346	2)	(347	1)	(360	8)	(361	120)	(362	66)
(363	29)	(364	7)	(365	2)	(377	3)	(378	1)
(379	1)	(393	1)	(407	1)	(408	1)	(435	3)
(451	5)	(463	2)	(464	1)				

NAME:12C_2929.8_1274EC17_[902; Melibiose (8TMS); alpha-D-Gal-(1,6)-D-Glc (8TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:293001-10-1

RI:2930

RT:18.009

NUM PEAKS: 124

(70	4)	(71	5)	(72	10)	(73	1000)	(74	85)
(75	81)	(76	4)	(77	6)	(79	3)	(81	20)
(83	6)	(85	5)	(87	5)	(89	8)	(97	4)
(99	5)	(101	14)	(102	4)	(103	136)	(104	13)
(105	6)	(109	7)	(111	4)	(113	7)	(115	5)
(116	11)	(117	40)	(118	4)	(119	5)	(127	5)
(129	146)	(130	17)	(131	28)	(132	4)	(133	51)
(134	7)	(135	5)	(139	3)	(141	4)	(142	4)
(143	27)	(144	4)	(145	6)	(147	276)	(148	43)
(149	31)	(150	4)	(151	3)	(153	5)	(155	11)
(156	3)	(157	19)	(158	3)	(159	4)	(161	5)
(163	4)	(169	38)	(170	8)	(171	6)	(173	4)
(175	5)	(177	6)	(181	3)	(183	4)	(189	26)
(190	10)	(191	223)	(192	39)	(193	18)	(201	3)
(203	12)	(204	808)	(205	166)	(206	70)	(207	18)
(208	3)	(215	5)	(217	159)	(218	37)	(219	17)
(220	3)	(221	21)	(222	5)	(223	3)	(229	6)
(230	24)	(231	14)	(232	4)	(233	5)	(239	3)
(242	3)	(243	25)	(244	7)	(245	7)	(246	3)
(255	3)	(257	4)	(265	6)	(271	14)	(272	3)
(291	9)	(292	3)	(293	9)	(295	3)	(304	6)
(305	24)	(306	9)	(307	4)	(317	4)	(318	14)
(319	12)	(320	4)	(331	5)	(332	8)	(333	4)
(343	7)	(344	3)	(345	5)	(361	29)	(362	11)
(363	5)	(433	16)	(434	8)	(435	5)		

NAME:12C_3337.9_1191EC10_[700; Ergosta-5,7-dien-3-ol]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:334001-10-1

RI:3338

RT:19.741

NUM PEAKS: 90

(70	66)	(71	155)	(73	1000)	(74	85)	(75	887)
(76	70)	(77	108)	(81	244)	(83	108)	(89	18)
(90	13)	(91	157)	(93	130)	(94	21)	(95	155)
(97	52)	(100	17)	(101	47)	(105	118)	(107	68)
(109	72)	(111	20)	(115	78)	(116	29)	(117	80)
(119	132)	(121	45)	(123	21)	(128	65)	(129	198)
(130	44)	(131	160)	(132	32)	(133	57)	(135	27)
(141	57)	(142	37)	(143	165)	(144	73)	(145	129)
(146	37)	(149	20)	(151	19)	(153	20)	(154	14)
(155	91)	(156	31)	(157	88)	(158	51)	(159	85)
(160	12)	(161	29)	(165	29)	(167	18)	(168	15)
(169	55)	(170	21)	(171	63)	(172	18)	(173	27)

196

(180	10)	(181	27)	(183	45)	(185	40)	(187	18)
(193	28)	(195	21)	(196	16)	(197	51)	(200	16)
(201	23)	(207	44)	(211	52)	(212	17)	(213	24)
(221	58)	(222	21)	(225	17)	(239	25)	(242	13)
(251	17)	(253	20)	(339	51)	(340	23)	(341	12)
(365	61)	(366	22)	(371	12)	(380	20)	(471	14)

NAME:12C_3350.3_1274EC11_[692; Ergosta-7,22-dien-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335001-10-1

RI:3350

RT:19.858

NUM PEAKS: 159

(70	48)	(73	599)	(74	60)	(75	1000)	(76	89)
(77	162)	(78	65)	(79	292)	(80	38)	(81	278)
(82	29)	(83	118)	(86	22)	(87	26)	(89	39)
(91	298)	(92	55)	(93	223)	(94	59)	(95	174)
(97	22)	(101	35)	(103	68)	(104	19)	(105	281)
(106	53)	(107	280)	(108	54)	(109	83)	(114	26)
(115	103)	(116	23)	(117	131)	(118	13)	(119	152)
(120	50)	(121	120)	(123	41)	(124	36)	(127	26)
(128	36)	(129	110)	(130	34)	(131	159)	(132	59)
(133	144)	(134	47)	(135	55)	(141	29)	(142	34)
(143	77)	(144	28)	(145	154)	(146	67)	(147	254)
(148	44)	(149	55)	(150	97)	(151	23)	(153	18)
(155	48)	(156	20)	(157	86)	(159	143)	(160	45)
(161	49)	(164	58)	(169	63)	(171	75)	(172	24)
(173	62)	(174	22)	(175	33)	(177	21)	(183	35)
(185	62)	(186	29)	(187	32)	(188	13)	(189	37)
(195	18)	(197	23)	(199	45)	(201	33)	(202	27)
(203	22)	(205	22)	(209	30)	(210	18)	(211	70)
(213	92)	(216	21)	(219	16)	(220	20)	(222	22)
(226	19)	(227	91)	(228	27)	(232	15)	(239	22)
(241	14)	(248	20)	(251	20)	(253	101)	(254	25)
(267	24)	(281	50)	(282	33)	(283	22)	(284	17)
(290	13)	(295	17)	(301	20)	(303	11)	(307	21)
(314	16)	(315	18)	(321	12)	(329	21)	(330	16)
(342	17)	(343	272)	(344	122)	(345	40)	(360	15)
(365	25)	(366	16)	(371	35)	(372	25)	(375	15)
(378	23)	(380	18)	(386	91)	(387	55)	(388	25)
(389	13)	(404	21)	(417	18)	(433	20)	(443	15)
(444	16)	(446	14)	(455	37)	(456	14)	(457	13)
(470	22)	(471	19)	(481	13)	(486	17)	(492	13)
(504	18)	(509	13)	(513	16)	(520	16)	(545	7)
(546	11)	(569	9)	(580	5)	(592	4)		

NAME:12C_3358.2_1191EC08_[693; Ergost-7-en-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:335002-10-1

RI:3358

RT:19.826

NUM PEAKS: 48

(71	242)	(73	477)	(75	1000)	(76	93)	(79	205)
(81	185)	(83	74)	(91	269)	(92	92)	(93	167)
(94	47)	(95	217)	(96	51)	(97	68)	(105	281)
(106	64)	(107	179)	(108	54)	(109	80)	(111	23)
(117	104)	(119	154)	(120	45)	(121	86)	(123	35)
(128	32)	(131	153)	(133	113)	(134	43)	(143	40)
(145	123)	(147	174)	(159	82)	(161	67)	(173	29)
(201	39)	(213	147)	(214	40)	(229	53)	(255	159)

197

(256 39) (273 19) (306 27) (307 19) (367 21)
 (471 15) (472 68) (473 40)

NAME:12C_3401.9_1274EC11_[805; 4,4-Dimethylcholesta-8,24-dien-3-ol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:340002-10-1

RI:3402

RT:20.078

NUM PEAKS: 112

(73 1000) (74 69) (75 649) (79 223) (81 364)
 (82 80) (87 36) (89 31) (91 278) (92 47)
 (93 269) (94 53) (95 377) (104 17) (105 290)
 (106 59) (107 286) (108 56) (109 265) (117 147)
 (119 264) (120 73) (121 183) (122 80) (123 130)
 (124 31) (128 35) (129 273) (131 178) (132 120)
 (133 228) (134 116) (135 775) (136 181) (137 84)
 (143 115) (144 54) (145 235) (146 128) (148 68)
 (149 188) (150 29) (152 34) (154 12) (156 29)
 (157 112) (158 33) (159 149) (160 66) (161 137)
 (162 40) (163 85) (169 26) (171 101) (172 31)
 (173 126) (174 75) (175 140) (176 38) (177 50)
 (183 41) (185 67) (186 29) (187 144) (188 61)
 (189 58) (190 29) (197 24) (199 61) (200 17)
 (201 49) (203 58) (211 62) (213 30) (215 48)
 (216 29) (225 69) (226 29) (229 50) (231 16)
 (241 113) (242 20) (243 65) (255 23) (257 36)
 (258 80) (259 27) (260 9) (278 14) (295 39)
 (296 27) (325 24) (326 23) (351 42) (366 12)
 (379 87) (380 53) (394 47) (396 17) (402 21)
 (467 15) (471 30) (474 11) (484 76) (485 71)
 (486 22) (491 23) (513 31) (540 16) (571 8)
 (590 9) (592 4)

NAME:12C_3487.5_1191EC08_[568; 2,3-Dihexadecanoylglycerol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:349001-10-1

RI:3488

RT:20.373

NUM PEAKS: 103

(70 57) (73 1000) (74 42) (75 286) (79 113)
 (81 88) (83 102) (84 41) (86 8) (91 29)
 (95 138) (97 49) (98 64) (101 46) (102 23)
 (103 242) (104 27) (105 18) (106 20) (107 20)
 (109 105) (115 33) (116 21) (117 84) (123 15)
 (126 7) (128 25) (129 629) (130 84) (131 115)
 (134 12) (135 41) (139 9) (142 13) (143 19)
 (145 456) (146 66) (147 26) (148 11) (149 32)
 (157 22) (159 9) (167 11) (168 21) (173 28)
 (174 10) (178 15) (182 18) (183 122) (184 7)
 (189 37) (193 33) (194 27) (201 27) (208 6)
 (219 29) (220 19) (224 24) (227 5) (237 13)
 (239 16) (243 5) (255 9) (257 194) (258 35)
 (259 19) (273 57) (274 16) (275 15) (277 9)
 (295 14) (296 10) (297 9) (300 7) (311 13)
 (312 13) (313 100) (314 16) (315 23) (327 25)
 (328 14) (329 30) (347 6) (348 6) (371 18)
 (384 11) (385 32) (390 5) (409 17) (424 11)
 (428 6) (433 28) (434 31) (469 11) (474 12)
 (538 7) (551 18) (556 6) (569 17) (572 15)
 (578 18) (579 10) (586 8)

NAME:12C_3301.9_1274EC11_[674; Ergosterol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:331001-10-1

RI:3302

RT:19.651

NUM PEAKS: 335

(70 165)	(71 742)	(72 81)	(73 1000)	(74 130)
(75 788)	(76 91)	(77 121)	(79 95)	(80 18)
(81 367)	(82 46)	(83 329)	(84 153)	(85 340)
(86 21)	(87 23)	(88 3)	(89 52)	(90 27)
(91 132)	(93 113)	(95 285)	(96 79)	(97 133)
(98 50)	(99 141)	(100 43)	(101 51)	(102 27)
(103 261)	(104 11)	(105 102)	(106 47)	(107 82)
(108 11)	(109 80)	(110 36)	(111 44)	(112 34)
(113 76)	(115 111)	(116 69)	(117 198)	(118 39)
(119 107)	(120 25)	(121 73)	(122 20)	(123 42)
(124 23)	(125 63)	(126 31)	(127 63)	(128 71)
(129 969)	(130 185)	(131 357)	(132 69)	(133 123)
(135 25)	(136 25)	(137 58)	(139 27)	(140 3)
(141 134)	(142 73)	(143 198)	(144 70)	(145 990)
(146 151)	(147 55)	(151 5)	(152 30)	(153 30)
(154 64)	(155 379)	(156 70)	(157 204)	(158 62)
(159 138)	(160 43)	(161 18)	(162 9)	(163 7)
(165 53)	(166 13)	(167 48)	(168 24)	(169 114)
(170 29)	(171 93)	(172 35)	(173 17)	(174 6)
(176 13)	(177 11)	(178 16)	(180 26)	(181 83)
(182 38)	(183 98)	(184 31)	(185 62)	(187 24)
(188 42)	(189 74)	(190 16)	(191 21)	(193 6)
(194 10)	(195 76)	(196 37)	(197 79)	(198 22)
(199 72)	(200 25)	(201 35)	(207 26)	(209 42)
(210 45)	(211 89)	(212 32)	(213 76)	(214 40)
(215 25)	(216 12)	(218 18)	(219 7)	(222 16)
(223 37)	(224 24)	(225 27)	(226 14)	(227 37)
(228 25)	(229 376)	(230 86)	(231 27)	(232 7)
(235 15)	(237 52)	(238 33)	(239 53)	(240 18)
(241 3)	(243 9)	(245 31)	(246 22)	(247 16)
(248 16)	(250 9)	(251 33)	(252 16)	(253 126)
(254 39)	(255 27)	(257 11)	(259 17)	(260 9)
(261 12)	(264 8)	(266 15)	(267 5)	(268 3)
(271 21)	(274 19)	(275 24)	(276 20)	(277 35)
(278 21)	(279 16)	(280 5)	(283 15)	(285 9)
(286 9)	(291 17)	(292 6)	(293 10)	(294 4)
(297 7)	(298 10)	(299 11)	(300 7)	(301 71)
(302 27)	(303 7)	(305 6)	(306 8)	(307 40)
(308 21)	(309 6)	(313 97)	(314 40)	(315 8)
(319 10)	(320 10)	(322 18)	(323 12)	(325 9)
(326 13)	(327 37)	(328 20)	(329 29)	(330 16)
(332 14)	(333 36)	(334 6)	(336 13)	(337 64)
(338 16)	(341 21)	(345 5)	(346 18)	(347 10)
(348 10)	(349 3)	(350 14)	(351 7)	(352 24)
(353 11)	(359 3)	(360 14)	(361 15)	(362 25)
(363 81)	(364 24)	(365 3)	(366 10)	(367 13)
(370 3)	(371 5)	(373 11)	(377 17)	(378 31)
(379 5)	(380 12)	(381 19)	(382 5)	(383 27)
(384 16)	(385 27)	(386 7)	(388 3)	(391 14)
(395 13)	(397 11)	(401 13)	(402 3)	(408 6)
(409 4)	(410 18)	(414 3)	(417 7)	(422 16)
(425 7)	(426 21)	(427 21)	(429 5)	(432 10)
(439 12)	(440 27)	(442 11)	(443 9)	(446 11)

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(447	13)	(449	21)	(450	29)	(453	3)	(456	6)
(459	6)	(463	3)	(465	12)	(466	42)	(467	25)
(468	38)	(469	35)	(470	5)	(471	14)	(472	15)
(473	4)	(475	31)	(476	24)	(480	13)	(489	23)
(490	4)	(491	8)	(494	5)	(495	20)	(497	14)
(498	8)	(500	16)	(501	3)	(502	7)	(503	25)
(508	7)	(509	12)	(511	5)	(512	8)	(514	16)
(515	10)	(516	10)	(518	11)	(521	17)	(522	15)
(524	12)	(525	11)	(526	4)	(527	4)	(528	13)
(535	26)	(538	4)	(540	16)	(542	14)	(543	21)
(544	17)	(545	5)	(550	3)	(551	5)	(553	4)
(556	10)	(559	5)	(564	3)	(569	5)	(573	3)
(575	7)	(580	10)	(583	9)	(585	6)	(589	9)
(590	10)	(593	5)	(595	4)	(597	5)	(598	7)

NAME:12C_3183.2_1160EC23_[748; D-Sedoheptulose-7-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:318001-10-1

RI:3183

RT:19.137

NUM PEAKS: 111

(72	7)	(73	1000)	(74	84)	(81	30)	(85	8)
(87	4)	(101	10)	(103	105)	(104	6)	(109	15)
(113	17)	(116	8)	(117	37)	(118	5)	(127	6)
(129	140)	(130	16)	(131	26)	(132	7)	(133	54)
(134	7)	(135	6)	(141	4)	(142	8)	(143	24)
(145	8)	(147	322)	(148	49)	(149	36)	(151	3)
(153	7)	(155	28)	(156	4)	(157	15)	(169	46)
(170	8)	(171	9)	(173	6)	(175	4)	(181	3)
(183	10)	(189	26)	(191	38)	(199	4)	(203	7)
(204	42)	(205	20)	(206	6)	(208	14)	(209	9)
(211	33)	(212	4)	(213	4)	(217	93)	(218	21)
(219	10)	(225	5)	(227	14)	(228	4)	(231	9)
(233	5)	(242	23)	(243	45)	(244	13)	(245	10)
(253	4)	(255	4)	(257	4)	(269	3)	(270	22)
(271	200)	(272	50)	(273	21)	(291	7)	(293	3)
(294	3)	(298	6)	(299	80)	(300	22)	(301	11)
(302	4)	(305	7)	(314	10)	(315	225)	(316	65)
(317	34)	(318	8)	(319	7)	(341	11)	(343	6)
(357	11)	(358	5)	(360	3)	(361	32)	(362	12)
(363	6)	(372	4)	(386	10)	(387	78)	(388	33)
(389	18)	(422	3)	(423	23)	(424	5)	(431	3)
(454	3)	(484	3)	(512	6)	(513	32)	(514	20)
(515	10)								

NAME:12C_2723.7_1160EC23_[777; Fructose-6-phosphate methoxyamine (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:272001-10-1

RI:2724

RT:17.023

NUM PEAKS: 75

(73	1000)	(74	78)	(89	58)	(90	7)	(91	10)
(101	64)	(121	7)	(127	7)	(129	155)	(133	57)
(135	29)	(140	9)	(142	112)	(143	18)	(151	18)
(165	5)	(173	74)	(174	38)	(180	8)	(181	18)
(193	12)	(195	26)	(207	20)	(211	84)	(212	11)
(214	6)	(217	158)	(218	22)	(225	66)	(226	14)
(227	23)	(228	14)	(236	16)	(269	10)	(283	16)
(285	12)	(298	13)	(299	334)	(300	83)	(301	35)
(313	14)	(314	19)	(315	343)	(316	95)	(317	41)

200

(318	10)	(328	5)	(341	8)	(342	5)	(354	20)
(357	43)	(358	13)	(379	3)	(386	35)	(387	255)
(388	100)	(389	56)	(390	11)	(394	6)	(410	3)
(414	13)	(449	5)	(451	15)	(453	6)	(454	3)
(459	21)	(460	6)	(461	9)	(474	5)	(542	5)
(543	4)	(544	10)	(545	9)	(546	6)	(558	3)

NAME:12C_2578.1_1274EC11_[734; 1-Monooleoylglycerol (2TMS); 1-Monohexadecenoylglycerol (1TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:258001-10-1

RI:2578

RT:16.266

NUM PEAKS: 108

(70	43)	(71	35)	(72	24)	(73	1000)	(74	89)
(75	313)	(76	15)	(77	38)	(79	66)	(80	23)
(81	185)	(82	42)	(83	124)	(84	32)	(85	27)
(89	40)	(91	22)	(93	50)	(94	18)	(95	108)
(96	33)	(97	79)	(98	48)	(99	32)	(100	8)
(101	139)	(102	18)	(103	308)	(104	30)	(105	33)
(106	6)	(107	31)	(108	14)	(109	50)	(110	12)
(111	45)	(112	12)	(113	24)	(115	23)	(116	79)
(117	133)	(118	20)	(119	31)	(120	14)	(121	53)
(122	10)	(123	40)	(124	6)	(125	16)	(129	580)
(130	102)	(131	154)	(132	49)	(133	124)	(134	27)
(135	67)	(136	17)	(137	35)	(139	10)	(145	52)
(146	40)	(147	444)	(148	75)	(149	84)	(150	14)
(151	20)	(152	7)	(153	13)	(159	6)	(161	9)
(162	4)	(163	24)	(165	16)	(171	6)	(175	20)
(176	9)	(187	14)	(188	19)	(192	9)	(201	90)
(202	20)	(203	127)	(205	58)	(206	10)	(215	23)
(219	34)	(220	6)	(221	14)	(236	15)	(237	53)
(238	12)	(243	7)	(244	7)	(255	6)	(257	40)
(258	20)	(272	5)	(279	22)	(286	13)	(311	11)
(339	7)	(369	106)	(370	46)	(371	17)	(382	19)
(457	17)	(458	14)	(475	3)				

NAME:12C_2386.9_1160EC23_[928; Glucopyranose-6-phosphate (6TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:239001-10-1

RI:2387

RT:15.242

NUM PEAKS: 78

(72	12)	(73	1000)	(74	84)	(75	100)	(81	17)
(87	3)	(99	4)	(101	20)	(111	6)	(113	18)
(115	6)	(116	9)	(127	4)	(129	153)	(130	15)
(131	24)	(133	58)	(134	6)	(135	9)	(143	15)
(147	180)	(148	25)	(149	21)	(151	5)	(155	10)
(161	4)	(169	10)	(181	6)	(189	25)	(190	5)
(191	46)	(192	7)	(193	8)	(195	5)	(204	221)
(205	43)	(206	16)	(207	12)	(208	3)	(211	37)
(212	5)	(217	57)	(219	5)	(225	9)	(227	9)
(231	5)	(242	5)	(243	12)	(247	6)	(253	4)
(269	5)	(270	7)	(271	18)	(272	4)	(283	3)
(285	3)	(298	4)	(299	110)	(300	29)	(301	14)
(314	4)	(315	40)	(316	11)	(317	8)	(345	8)
(357	36)	(358	11)	(359	5)	(369	3)	(370	20)
(371	7)	(372	3)	(373	3)	(386	14)	(387	120)
(388	48)	(389	28)	(390	7)				

201

NAME:12C_2310.0_1191EC10_Fructose-6-phosphate methoxyamine (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:232002-10-1

RI:2310

RT:14.783

NUM PEAKS: 127

(70	8)	(71	11)	(72	15)	(73	1000)	(74	90)
(75	89)	(76	4)	(77	8)	(81	4)	(82	3)
(83	7)	(84	28)	(85	11)	(87	4)	(88	3)
(89	47)	(90	5)	(91	4)	(93	3)	(95	3)
(97	5)	(98	4)	(99	6)	(100	7)	(101	32)
(102	6)	(103	73)	(104	9)	(105	6)	(111	4)
(113	7)	(114	11)	(115	9)	(116	11)	(117	21)
(118	3)	(119	7)	(126	5)	(127	5)	(128	3)
(129	65)	(130	7)	(131	18)	(132	3)	(133	56)
(134	7)	(135	11)	(137	3)	(141	3)	(142	5)
(143	7)	(147	129)	(148	21)	(149	14)	(151	4)
(152	4)	(155	4)	(156	4)	(157	5)	(159	3)
(163	5)	(169	4)	(172	5)	(173	5)	(180	3)
(181	6)	(182	4)	(183	3)	(189	7)	(190	3)
(191	11)	(193	6)	(195	7)	(196	3)	(197	3)
(204	10)	(205	8)	(206	3)	(207	11)	(208	3)
(209	4)	(211	29)	(212	6)	(213	3)	(214	3)
(217	81)	(218	19)	(219	7)	(221	5)	(225	11)
(226	3)	(227	8)	(232	4)	(243	5)	(244	4)
(245	4)	(260	3)	(270	3)	(271	3)	(283	3)
(285	5)	(286	3)	(298	5)	(299	64)	(300	23)
(301	11)	(302	4)	(313	3)	(314	8)	(315	105)
(316	31)	(317	15)	(318	5)	(319	3)	(341	5)
(342	3)	(355	3)	(356	4)	(357	15)	(358	5)
(359	3)	(373	3)	(403	5)	(458	3)	(459	9)
(460	4)	(461	3)						

NAME:12C_2257.2_1160EC23_[715; Erythritol (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:226001-10-1

RI:2257

RT:14.556

NUM PEAKS: 143

(70	24)	(72	14)	(73	1000)	(74	61)	(75	94)
(76	5)	(80	4)	(82	13)	(83	9)	(84	290)
(85	22)	(86	22)	(88	3)	(89	36)	(90	3)
(94	4)	(96	3)	(99	8)	(100	17)	(101	8)
(102	8)	(103	227)	(104	20)	(105	11)	(108	3)
(111	12)	(112	3)	(113	7)	(114	8)	(115	4)
(116	24)	(117	66)	(118	8)	(119	6)	(123	3)
(126	3)	(127	3)	(128	11)	(129	34)	(130	10)
(131	18)	(132	6)	(133	45)	(134	5)	(135	6)
(140	4)	(141	6)	(142	33)	(143	20)	(144	43)
(145	9)	(146	4)	(147	210)	(148	32)	(149	20)
(153	3)	(154	3)	(155	4)	(157	12)	(158	11)
(159	4)	(161	3)	(163	4)	(167	4)	(168	6)
(169	3)	(170	7)	(171	4)	(172	14)	(173	15)
(174	53)	(175	11)	(176	3)	(180	3)	(182	4)
(183	8)	(184	3)	(186	11)	(187	5)	(188	5)
(189	18)	(190	3)	(191	9)	(198	3)	(200	7)
(201	8)	(202	30)	(203	6)	(204	13)	(205	31)
(206	7)	(207	3)	(213	6)	(214	5)	(216	3)
(217	93)	(218	20)	(219	7)	(221	4)	(225	12)
(226	3)	(232	3)	(242	5)	(243	3)	(244	4)

202

(256	5)	(257	9)	(258	4)	(260	3)	(268	4)
(269	3)	(270	4)	(271	5)	(277	6)	(300	3)
(307	9)	(308	3)	(316	3)	(330	12)	(331	8)
(332	3)	(342	5)	(343	4)	(367	4)	(372	3)
(373	34)	(374	19)	(375	8)	(376	3)	(403	4)
(404	3)	(437	4)	(447	9)	(448	6)	(457	4)
(476	3)	(477	3)	(547	7)	(548	6)	(550	3)
(551	7)	(552	6)	(553	3)				

NAME: 12C 2718.4 1313EC43 [824; D-Sedoheptulose-7-phosphate (7TMS)]

COMMENTS: Kopka J, MPIMP, Dept. Willmitzer

CASNO: 272002-10-1

RI: 2718

RT: 16.521

NUM PEAKS: 469

(70	2)	(72	15)	(73	1000)	(74	86)	(75	58)
(76	3)	(77	6)	(79	1)	(80	1)	(81	6)
(82	6)	(84	2)	(86	3)	(87	6)	(88	3)
(89	24)	(90	3)	(91	3)	(92	2)	(93	3)
(94	2)	(95	1)	(96	2)	(98	4)	(100	6)
(101	39)	(102	6)	(103	47)	(104	6)	(105	10)
(106	3)	(107	7)	(108	2)	(109	4)	(110	1)
(111	4)	(112	2)	(113	7)	(114	6)	(115	11)
(116	18)	(117	22)	(118	3)	(119	8)	(120	2)
(121	6)	(122	3)	(123	3)	(124	3)	(125	1)
(126	3)	(127	3)	(128	4)	(129	113)	(130	16)
(131	22)	(132	7)	(133	62)	(134	9)	(135	18)
(136	4)	(137	11)	(138	4)	(139	3)	(140	4)
(141	1)	(142	25)	(143	12)	(144	3)	(145	7)
(146	2)	(147	132)	(148	23)	(149	16)	(150	3)
(151	9)	(152	3)	(153	4)	(154	4)	(155	8)
(156	5)	(157	10)	(158	5)	(159	4)	(160	12)
(161	10)	(162	2)	(163	7)	(164	2)	(165	4)
(166	4)	(167	4)	(168	5)	(169	13)	(170	6)
(171	6)	(172	4)	(173	25)	(174	5)	(175	5)
(176	2)	(177	2)	(178	2)	(179	4)	(180	7)
(181	12)	(182	6)	(183	7)	(184	3)	(185	3)
(186	3)	(187	2)	(188	2)	(189	16)	(190	6)
(191	104)	(192	18)	(193	19)	(194	4)	(195	12)
(196	8)	(197	5)	(198	4)	(199	8)	(200	4)
(201	2)	(202	2)	(203	5)	(204	103)	(205	19)
(206	7)	(207	18)	(208	5)	(209	7)	(210	5)
(211	58)	(212	10)	(213	7)	(214	2)	(215	4)
(216	4)	(217	121)	(218	31)	(219	15)	(220	2)
(221	3)	(222	1)	(223	1)	(224	2)	(225	25)
(226	6)	(227	16)	(228	7)	(229	4)	(230	4)
(231	6)	(232	2)	(233	2)	(234	2)	(235	1)
(236	8)	(237	2)	(238	1)	(239	1)	(240	3)
(241	5)	(242	4)	(243	16)	(244	3)	(245	3)
(246	1)	(247	4)	(248	1)	(249	1)	(250	2)
(251	2)	(252	2)	(253	4)	(254	4)	(255	4)
(256	2)	(257	3)	(258	2)	(259	4)	(260	2)
(261	3)	(262	1)	(263	1)	(264	2)	(265	2)
(266	3)	(267	3)	(268	5)	(269	5)	(270	5)
(271	5)	(272	4)	(273	2)	(274	2)	(275	2)
(276	1)	(277	3)	(278	2)	(279	2)	(280	1)
(281	1)	(282	3)	(283	7)	(284	4)	(285	8)
(286	4)	(287	2)	(289	4)	(290	2)	(291	3)
(292	3)	(294	1)	(295	1)	(297	2)	(298	12)
(299	132)	(300	41)	(301	20)	(302	3)	(303	2)

203

(304	4)	(305	6)	(306	4)	(307	3)	(308	2)
(309	2)	(310	1)	(311	2)	(312	2)	(313	4)
(314	14)	(315	128)	(316	36)	(317	20)	(318	5)
(320	1)	(322	2)	(323	1)	(325	1)	(326	1)
(327	2)	(328	2)	(329	3)	(330	3)	(331	2)
(332	2)	(335	2)	(337	1)	(339	2)	(340	2)
(341	6)	(342	2)	(343	2)	(345	3)	(346	2)
(347	1)	(348	3)	(349	2)	(350	1)	(351	1)
(352	3)	(353	4)	(354	12)	(355	5)	(356	7)
(357	21)	(358	8)	(359	4)	(360	5)	(361	29)
(362	9)	(363	6)	(364	4)	(365	3)	(366	1)
(367	2)	(368	2)	(369	1)	(370	3)	(371	3)
(372	2)	(373	4)	(374	2)	(375	2)	(376	2)
(377	1)	(380	1)	(381	2)	(382	2)	(383	1)
(384	2)	(385	3)	(386	20)	(387	81)	(388	32)
(389	15)	(390	4)	(391	1)	(392	2)	(393	2)
(394	1)	(395	2)	(396	3)	(397	1)	(398	2)
(399	1)	(400	1)	(401	2)	(402	1)	(403	2)
(404	2)	(405	1)	(406	1)	(408	1)	(409	1)
(410	2)	(411	2)	(413	4)	(414	11)	(415	4)
(416	4)	(417	2)	(418	3)	(419	1)	(420	1)
(421	1)	(422	1)	(423	2)	(424	2)	(425	1)
(426	1)	(427	1)	(428	1)	(429	1)	(430	2)
(431	1)	(432	2)	(433	2)	(434	3)	(435	1)
(436	3)	(437	4)	(438	3)	(439	1)	(440	1)
(441	1)	(442	3)	(443	2)	(444	1)	(445	1)
(446	1)	(448	2)	(449	2)	(450	4)	(451	5)
(452	4)	(453	3)	(454	3)	(455	1)	(456	1)
(457	1)	(458	4)	(459	12)	(460	6)	(461	3)
(462	1)	(463	2)	(466	1)	(467	1)	(468	1)
(469	1)	(470	2)	(471	1)	(472	2)	(473	1)
(475	1)	(476	2)	(480	2)	(481	2)	(482	1)
(483	1)	(484	2)	(485	1)	(486	3)	(487	2)
(489	2)	(490	1)	(491	2)	(492	2)	(493	1)
(494	1)	(495	2)	(496	1)	(498	2)	(499	2)
(500	2)	(502	2)	(503	2)	(504	1)	(505	1)
(506	2)	(507	1)	(508	2)	(509	2)	(511	2)
(512	2)	(513	1)	(514	1)	(515	1)	(516	2)
(517	1)	(518	2)	(519	2)	(521	1)	(522	3)
(523	2)	(524	1)	(525	3)	(526	2)	(527	3)
(530	2)	(531	1)	(533	1)	(534	3)	(535	1)
(536	1)	(537	1)	(538	3)	(539	2)	(540	2)
(541	2)	(542	2)	(543	1)	(544	2)	(545	3)
(546	2)	(547	1)	(548	2)	(549	1)	(550	1)
(551	1)	(553	1)	(554	1)	(555	1)	(556	2)
(557	1)	(558	1)	(559	1)	(560	1)	(561	1)
(562	1)	(563	1)	(564	1)	(565	1)	(566	1)
(571	1)	(572	1)	(573	1)	(574	1)	(575	1)
(577	1)	(578	1)	(581	1)	(588	1)		

NAME:12C 2347.2_1313EC43_Glucose-6-phosphate methoxyamine {BP} (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:235002-10-1

RI:2347

RT: 14.555

NUM PEAKS: 146

(72	15)	(73	1000)	(74	81)	(75	103)	(76	7)
(77	11)	(79	7)	(80	3)	(81	6)	(86	4)
(87	4)	(88	3)	(89	46)	(90	5)	(91	8)
(92	2)	(93	3)	(95	4)	(97	3)	(98	3)

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(100	8)	(101	37)	(102	9)	(103	48)	(104	4)
(105	14)	(106	5)	(107	3)	(108	2)	(109	2)
(114	8)	(115	11)	(116	19)	(118	2)	(119	8)
(121	3)	(129	69)	(130	16)	(131	30)	(133	66)
(134	10)	(135	14)	(136	2)	(137	4)	(138	2)
(142	2)	(143	11)	(144	2)	(145	7)	(146	2)
(147	132)	(148	19)	(149	18)	(150	4)	(151	5)
(154	2)	(157	32)	(158	4)	(159	6)	(160	38)
(161	13)	(162	2)	(163	5)	(172	2)	(173	3)
(174	2)	(175	2)	(176	2)	(177	2)	(180	2)
(181	6)	(188	1)	(189	8)	(190	1)	(191	14)
(192	3)	(193	8)	(194	2)	(195	4)	(197	2)
(201	3)	(203	5)	(204	7)	(205	8)	(207	16)
(211	38)	(212	6)	(213	5)	(215	2)	(216	3)
(217	30)	(218	6)	(225	10)	(226	2)	(227	8)
(228	5)	(229	4)	(230	3)	(231	2)	(241	3)
(243	5)	(244	3)	(245	2)	(247	8)	(253	3)
(265	1)	(268	2)	(269	5)	(270	1)	(278	1)
(283	3)	(285	4)	(298	8)	(299	92)	(300	26)
(301	11)	(314	9)	(315	43)	(316	12)	(317	6)
(318	1)	(319	2)	(331	4)	(332	2)	(341	4)
(356	6)	(357	27)	(358	8)	(359	3)	(370	2)
(373	3)	(374	2)	(385	2)	(386	27)	(387	101)
(388	39)	(389	19)	(390	3)	(409	1)	(435	1)
(470	4)	(471	9)	(472	3)	(473	3)	(501	2)
(569	1)								

NAME:12C_2039.0_1313EC43_[607; Putrescine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:204003-10-1

RI:2039

RT: 12.763

NUM PEAKS: 219

(70	80)	(71	135)	(72	41)	(73	616)	(74	121)
(75	287)	(76	2)	(79	19)	(80	11)	(81	17)
(82	3)	(83	22)	(84	132)	(85	103)	(86	256)
(87	53)	(88	26)	(93	10)	(94	4)	(95	7)
(96	3)	(98	29)	(99	150)	(100	259)	(101	1)
(102	49)	(108	1)	(110	49)	(111	4)	(112	71)
(113	21)	(114	42)	(115	4)	(116	31)	(122	9)
(123	11)	(124	12)	(125	2)	(126	152)	(127	44)
(128	7)	(130	106)	(131	25)	(140	26)	(141	9)
(142	128)	(143	10)	(146	57)	(147	116)	(148	31)
(150	4)	(152	9)	(153	7)	(154	21)	(155	10)
(156	5)	(157	5)	(158	12)	(160	252)	(161	1)
(162	7)	(164	5)	(166	9)	(167	14)	(168	5)
(169	1)	(170	3)	(172	112)	(173	4)	(174	407)
(175	51)	(176	45)	(179	18)	(180	6)	(181	13)
(182	4)	(183	5)	(185	2)	(186	34)	(188	24)
(194	5)	(197	7)	(198	9)	(200	118)	(201	19)
(204	129)	(207	10)	(208	9)	(210	3)	(212	6)
(213	5)	(214	1000)	(215	205)	(216	97)	(231	9)
(232	4)	(233	3)	(239	9)	(240	12)	(241	4)
(242	1)	(245	3)	(246	28)	(250	6)	(251	3)
(252	12)	(253	1)	(257	3)	(258	13)	(259	2)
(261	5)	(266	11)	(267	5)	(268	27)	(269	18)
(270	5)	(272	3)	(276	1)	(280	7)	(281	1)
(282	3)	(283	12)	(287	5)	(288	49)	(289	13)
(291	11)	(292	21)	(295	3)	(305	1)	(311	17)
(319	30)	(320	4)	(321	6)	(324	2)	(325	5)

205

(330	9)	(331	2)	(332	2)	(334	4)	(336	7)
(339	17)	(352	9)	(353	2)	(355	15)	(356	10)
(358	1)	(360	1)	(361	6)	(363	2)	(367	1)
(372	14)	(374	8)	(375	61)	(376	48)	(377	18)
(381	3)	(395	14)	(398	2)	(407	2)	(412	2)
(416	2)	(420	2)	(425	8)	(430	3)	(435	1)
(439	2)	(443	1)	(444	3)	(448	8)	(452	4)
(454	2)	(455	2)	(456	6)	(457	9)	(458	6)
(461	4)	(462	8)	(465	4)	(467	7)	(469	3)
(471	4)	(474	12)	(475	21)	(476	9)	(478	13)
(479	5)	(482	4)	(483	6)	(484	6)	(488	5)
(489	3)	(493	15)	(494	2)	(497	15)	(501	10)
(502	2)	(504	1)	(505	4)	(506	2)	(513	7)
(525	2)	(526	3)	(527	7)	(530	7)	(538	1)
(547	2)	(550	4)	(552	7)	(563	3)	(566	1)
(571	2)	(575	11)	(580	5)	(583	6)	(586	5)
(589	2)	(590	1)	(592	6)	(595	4)		

NAME:12C_1476.2_1313EC75_Citramalic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:148001-10-1

RI:1476

RT: 8.471

NUM PEAKS: 38

(73	1000)	(74	89)	(75	222)	(76	14)	(85	40)
(86	6)	(115	117)	(116	15)	(117	41)	(131	33)
(133	83)	(134	10)	(143	17)	(144	8)	(147	404)
(148	65)	(149	70)	(150	8)	(151	5)	(157	14)
(163	29)	(164	5)	(185	18)	(190	8)	(203	33)
(205	6)	(219	3)	(221	14)	(231	32)	(233	26)
(247	141)	(248	31)	(259	33)	(260	7)	(261	4)
(321	16)	(322	6)	(349	10)				

NAME:12C_1735.8_1313EC75_Glycerol-2-phosphate (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174002-10-1

RI:1736

RT: 10.585

NUM PEAKS: 393

(70	9)	(71	14)	(72	24)	(73	1000)	(74	81)
(75	224)	(76	10)	(77	18)	(78	7)	(79	14)
(80	4)	(81	5)	(82	4)	(83	5)	(84	16)
(85	11)	(86	7)	(87	13)	(88	4)	(89	25)
(90	4)	(91	8)	(92	6)	(93	7)	(94	5)
(95	5)	(96	5)	(97	9)	(98	6)	(99	10)
(100	10)	(101	93)	(102	12)	(103	111)	(104	10)
(105	15)	(106	9)	(107	4)	(108	1)	(109	3)
(110	4)	(111	6)	(112	2)	(113	11)	(114	6)
(115	21)	(116	55)	(117	43)	(118	11)	(119	9)
(120	3)	(121	6)	(122	2)	(123	7)	(124	3)
(125	1)	(126	2)	(127	6)	(128	3)	(129	114)
(130	15)	(131	43)	(132	5)	(133	84)	(134	16)
(135	15)	(136	3)	(137	9)	(138	5)	(139	4)
(140	5)	(141	11)	(142	8)	(143	10)	(144	2)
(145	1)	(146	4)	(147	224)	(148	39)	(149	30)
(150	5)	(151	7)	(152	4)	(153	56)	(154	9)
(155	8)	(156	1)	(157	10)	(159	27)	(160	9)
(161	4)	(162	1)	(163	8)	(166	3)	(167	12)
(168	5)	(169	10)	(170	8)	(171	5)	(174	7)
(175	5)	(176	3)	(177	8)	(178	1)	(179	3)

206

(180	6)	(181	10)	(182	3)	(183	6)	(184	1)
(185	3)	(186	3)	(187	5)	(188	4)	(189	16)
(190	6)	(191	17)	(192	7)	(193	14)	(194	6)
(195	9)	(196	1)	(197	4)	(198	1)	(199	1)
(200	3)	(201	1)	(203	6)	(204	33)	(205	23)
(206	3)	(207	24)	(210	3)	(211	90)	(212	20)
(213	10)	(214	1)	(215	4)	(216	1)	(217	61)
(218	20)	(219	8)	(220	4)	(221	2)	(222	3)
(223	2)	(225	6)	(226	4)	(227	20)	(228	5)
(229	5)	(230	3)	(231	16)	(232	8)	(233	3)
(234	3)	(235	4)	(236	1)	(237	5)	(239	5)
(240	2)	(241	25)	(242	7)	(243	129)	(244	18)
(245	7)	(246	2)	(247	3)	(248	4)	(249	2)
(250	3)	(253	3)	(254	3)	(257	1)	(258	2)
(259	2)	(260	1)	(261	2)	(263	2)	(264	2)
(265	2)	(266	2)	(267	2)	(268	5)	(269	9)
(270	6)	(271	5)	(272	1)	(273	2)	(274	4)
(275	4)	(277	4)	(279	1)	(280	2)	(281	2)
(283	3)	(284	11)	(285	16)	(286	4)	(287	6)
(293	1)	(294	6)	(297	1)	(298	11)	(299	63)
(300	22)	(301	11)	(302	5)	(304	5)	(305	16)
(306	13)	(307	10)	(308	5)	(309	4)	(310	1)
(311	1)	(313	3)	(314	3)	(315	13)	(316	5)
(317	2)	(318	3)	(319	9)	(320	4)	(321	4)
(322	1)	(323	4)	(324	1)	(325	1)	(326	3)
(327	3)	(328	4)	(331	2)	(332	2)	(338	5)
(339	1)	(340	2)	(341	2)	(342	6)	(343	3)
(345	3)	(346	1)	(349	2)	(350	1)	(352	3)
(353	2)	(355	3)	(357	3)	(358	4)	(359	3)
(360	1)	(361	3)	(365	1)	(367	1)	(368	1)
(369	3)	(372	1)	(373	5)	(374	2)	(375	4)
(376	4)	(377	4)	(378	3)	(379	2)	(380	1)
(381	1)	(382	2)	(383	2)	(384	1)	(385	4)
(386	3)	(387	4)	(388	1)	(389	10)	(390	8)
(391	4)	(393	3)	(395	1)	(396	2)	(397	2)
(398	1)	(399	3)	(400	2)	(401	2)	(404	3)
(405	2)	(406	2)	(407	2)	(411	2)	(412	2)
(415	4)	(416	3)	(417	1)	(421	1)	(422	3)
(423	1)	(424	2)	(427	4)	(428	3)	(430	1)
(432	2)	(434	1)	(438	4)	(439	2)	(444	4)
(445	7)	(446	2)	(448	4)	(449	4)	(450	2)
(452	3)	(453	4)	(454	2)	(457	2)	(458	4)
(460	1)	(461	2)	(462	1)	(463	1)	(464	4)
(465	2)	(466	2)	(467	4)	(468	3)	(469	3)
(472	4)	(473	3)	(476	3)	(477	3)	(480	2)
(481	2)	(482	3)	(486	2)	(487	1)	(488	2)
(491	1)	(492	2)	(493	2)	(494	7)	(495	2)
(497	5)	(498	2)	(500	1)	(502	4)	(503	5)
(504	5)	(505	1)	(506	2)	(507	1)	(510	3)
(511	4)	(514	4)	(515	1)	(517	5)	(518	3)
(519	3)	(521	1)	(522	4)	(523	2)	(524	3)
(526	4)	(527	2)	(529	1)	(530	1)	(534	6)
(537	2)	(538	2)	(541	2)	(543	2)	(544	4)
(545	1)	(547	1)	(548	5)	(552	4)	(554	3)
(555	4)	(556	1)	(561	1)	(562	1)	(563	1)
(564	3)	(565	1)	(566	4)	(567	3)	(570	1)
(572	1)	(574	1)	(575	1)	(579	1)	(582	1)
(583	3)	(596	1)	(597	1)				

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NAME:12C_1761.3_1313EC75_[757; 2-Desoxy-pentos-3-ylose dimethoxyamine
(2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:176004-10-1

RI:1762

RT: 10.782

NUM PEAKS: 86

(73	1000)	(74	100)	(81	5)	(89	133)	(93	3)
(94	5)	(95	18)	(101	53)	(103	122)	(104	11)
(105	57)	(106	6)	(107	3)	(108	5)	(111	10)
(117	87)	(118	10)	(119	17)	(121	9)	(123	3)
(126	14)	(133	157)	(134	19)	(135	12)	(136	1)
(137	3)	(142	278)	(143	52)	(147	234)	(148	41)
(149	31)	(153	8)	(163	16)	(164	3)	(167	17)
(179	1)	(180	3)	(181	5)	(189	12)	(190	5)
(191	17)	(192	3)	(194	2)	(195	4)	(197	3)
(198	2)	(199	25)	(201	27)	(202	3)	(204	12)
(205	51)	(206	9)	(207	3)	(209	1)	(212	3)
(217	50)	(218	9)	(219	3)	(225	8)	(226	4)
(230	7)	(231	667)	(232	103)	(233	28)	(234	3)
(241	2)	(256	1)	(257	10)	(271	3)	(273	5)
(277	2)	(307	7)	(314	3)	(315	27)	(316	7)
(331	5)	(332	3)	(333	5)	(334	2)	(346	2)
(373	1)	(404	1)	(405	9)	(406	3)	(407	2)
(421	3)								

NAME:12C_1796.4_1313EC75_[646; 3-Deoxyglucitol (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:180001-10-1

RI:1796

RT: 11.055

NUM PEAKS: 263

(70	11)	(71	11)	(72	24)	(73	1000)	(74	90)
(75	119)	(76	9)	(77	4)	(79	1)	(80	4)
(81	5)	(82	6)	(83	2)	(84	42)	(85	18)
(87	7)	(88	5)	(89	70)	(90	7)	(91	6)
(92	1)	(93	8)	(94	4)	(95	110)	(96	10)
(97	4)	(98	14)	(99	11)	(100	10)	(101	45)
(102	7)	(103	123)	(104	12)	(105	92)	(106	9)
(107	5)	(108	3)	(109	2)	(110	3)	(111	11)
(112	7)	(113	6)	(114	1)	(115	9)	(116	22)
(117	67)	(118	9)	(119	11)	(120	2)	(121	7)
(122	3)	(123	10)	(125	3)	(126	21)	(127	8)
(128	3)	(129	26)	(130	7)	(131	28)	(132	6)
(133	77)	(134	9)	(135	8)	(136	3)	(137	2)
(138	3)	(139	7)	(140	4)	(141	4)	(142	21)
(143	14)	(144	4)	(145	4)	(146	3)	(147	192)
(148	29)	(149	26)	(150	3)	(151	4)	(152	3)
(153	8)	(155	4)	(156	15)	(157	7)	(158	17)
(159	6)	(160	2)	(161	2)	(162	1)	(163	8)
(164	2)	(165	2)	(166	2)	(167	22)	(168	7)
(169	5)	(170	4)	(172	2)	(173	3)	(175	4)
(177	2)	(179	2)	(180	1)	(181	3)	(182	2)
(183	6)	(184	4)	(185	3)	(186	7)	(187	3)
(189	10)	(191	20)	(192	3)	(193	2)	(194	3)
(195	4)	(196	2)	(198	2)	(199	90)	(200	17)
(201	29)	(202	6)	(203	2)	(204	10)	(205	44)
(206	8)	(209	2)	(210	1)	(211	2)	(212	5)
(213	3)	(214	2)	(215	2)	(216	11)	(217	55)
(218	11)	(219	5)	(221	1)	(223	1)	(225	7)

208

(226	2)	(227	2)	(228	5)	(229	2)	(230	5)
(231	105)	(232	17)	(233	5)	(235	1)	(236	1)
(241	1)	(242	2)	(243	9)	(244	2)	(245	1)
(248	1)	(249	1)	(253	1)	(254	1)	(255	2)
(256	2)	(257	7)	(261	1)	(266	1)	(268	1)
(269	3)	(270	2)	(271	2)	(273	5)	(274	2)
(275	1)	(277	3)	(278	2)	(285	2)	(287	1)
(288	1)	(289	1)	(290	1)	(291	1)	(296	1)
(299	2)	(300	2)	(302	2)	(304	1)	(305	1)
(306	2)	(307	12)	(308	4)	(309	2)	(314	2)
(315	21)	(316	6)	(317	2)	(318	3)	(319	1)
(323	1)	(327	1)	(329	1)	(330	1)	(331	4)
(332	2)	(333	6)	(334	2)	(335	1)	(336	1)
(337	1)	(342	1)	(344	1)	(346	2)	(347	1)
(351	2)	(352	1)	(358	1)	(359	1)	(361	1)
(365	1)	(367	1)	(376	1)	(381	1)	(399	1)
(402	1)	(404	2)	(405	5)	(406	2)	(412	1)
(414	1)	(420	1)	(421	2)	(422	1)	(424	1)
(425	1)	(428	1)	(432	1)	(439	1)	(455	1)
(456	1)	(462	1)	(465	1)	(475	1)	(479	1)
(480	1)	(495	1)	(502	1)	(504	1)	(510	1)
(516	1)	(517	1)	(520	1)	(523	1)	(524	1)
(528	1)	(529	2)	(531	1)	(542	1)	(543	1)
(545	1)	(547	1)	(548	1)	(552	1)	(560	1)
(566	1)	(571	1)	(590	1)				

NAME:12C_3380.0_1274EC11_Lanosta-8,24-dien-3-beta-ol (1TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:338001-10-1

RI:3380

RT:19.985

NUM PEAKS: 215

(70	99)	(72	17)	(73	1000)	(74	97)	(75	732)
(76	67)	(77	169)	(78	49)	(79	252)	(80	28)
(81	444)	(82	57)	(83	204)	(84	20)	(87	11)
(88	10)	(89	30)	(90	10)	(91	261)	(92	37)
(93	280)	(94	37)	(95	457)	(96	40)	(97	66)
(98	10)	(101	17)	(103	35)	(104	10)	(105	295)
(106	41)	(107	273)	(108	41)	(109	538)	(110	48)
(111	54)	(114	8)	(115	59)	(116	25)	(117	129)
(118	27)	(119	293)	(120	52)	(121	251)	(122	49)
(123	179)	(124	19)	(125	12)	(127	19)	(128	54)
(129	244)	(130	55)	(131	184)	(132	37)	(133	211)
(134	47)	(135	237)	(136	39)	(137	88)	(138	15)
(139	7)	(141	38)	(142	39)	(143	124)	(144	40)
(145	191)	(146	42)	(147	212)	(148	45)	(149	134)
(150	22)	(151	31)	(152	15)	(153	14)	(154	16)
(155	38)	(156	26)	(157	133)	(158	38)	(159	167)
(160	64)	(161	167)	(162	37)	(163	80)	(164	15)
(165	29)	(166	14)	(167	13)	(168	10)	(169	36)
(170	17)	(171	89)	(172	33)	(173	129)	(174	42)
(175	117)	(176	18)	(177	45)	(178	11)	(179	16)
(181	12)	(182	8)	(183	36)	(184	16)	(185	72)
(186	24)	(187	158)	(188	33)	(189	139)	(190	34)
(191	69)	(192	17)	(193	20)	(197	27)	(198	13)
(199	59)	(200	21)	(201	71)	(202	21)	(203	55)
(204	20)	(205	18)	(206	8)	(207	64)	(208	12)
(209	11)	(211	27)	(212	15)	(213	52)	(214	29)
(215	86)	(216	21)	(217	31)	(219	10)	(220	7)
(225	28)	(226	11)	(227	79)	(228	20)	(229	79)

209

(230	18)	(231	14)	(232	4)	(233	6)	(237	6)
(239	14)	(240	8)	(241	136)	(242	33)	(243	36)
(244	12)	(245	10)	(253	15)	(254	8)	(255	57)
(256	17)	(257	34)	(258	11)	(259	9)	(265	10)
(266	9)	(267	18)	(269	25)	(270	12)	(271	17)
(272	22)	(273	11)	(281	29)	(282	11)	(283	27)
(284	7)	(285	11)	(286	5)	(295	9)	(297	16)
(298	8)	(299	6)	(309	15)	(310	6)	(311	27)
(312	11)	(317	5)	(319	6)	(323	15)	(325	10)
(328	6)	(331	9)	(332	6)	(335	4)	(349	5)
(350	11)	(351	15)	(352	9)	(386	8)	(389	3)
(393	276)	(394	162)	(395	38)	(408	4)	(413	10)
(427	4)	(450	6)	(477	4)	(482	11)	(483	70)
(484	72)	(485	27)	(486	9)	(487	5)	(497	14)
(498	77)	(499	67)	(500	28)	(501	10)	(506	6)

NAME:12C_3081.9_1160EC23_[808; Adenosine-5'-monophosphate (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:308001-10-1

RI:3082

RT:18.685

NUM PEAKS: 174

(70	5)	(71	5)	(72	18)	(73	1000)	(74	93)
(75	110)	(76	7)	(77	11)	(80	3)	(81	29)
(82	3)	(85	8)	(86	4)	(87	5)	(89	7)
(92	3)	(93	3)	(94	5)	(95	7)	(97	12)
(98	4)	(99	14)	(100	3)	(101	27)	(102	6)
(103	12)	(105	4)	(107	3)	(108	29)	(109	5)
(111	8)	(113	18)	(114	3)	(115	18)	(116	11)
(117	11)	(118	3)	(119	14)	(120	3)	(121	6)
(125	9)	(126	3)	(127	11)	(129	66)	(130	9)
(131	20)	(132	5)	(133	78)	(134	12)	(135	85)
(136	80)	(137	12)	(139	3)	(140	24)	(141	15)
(142	18)	(143	26)	(144	4)	(145	7)	(146	3)
(147	143)	(148	30)	(149	24)	(150	6)	(151	9)
(153	12)	(154	3)	(155	5)	(156	3)	(157	6)
(158	3)	(159	4)	(160	3)	(161	4)	(162	3)
(163	3)	(164	40)	(165	8)	(167	6)	(168	3)
(169	469)	(170	67)	(171	44)	(172	6)	(173	4)
(174	4)	(175	4)	(177	3)	(178	3)	(179	4)
(181	12)	(183	6)	(184	5)	(185	4)	(186	7)
(187	3)	(189	4)	(190	3)	(191	6)	(193	10)
(194	5)	(195	14)	(196	3)	(197	5)	(204	3)
(205	3)	(206	20)	(207	27)	(208	31)	(209	8)
(210	4)	(211	83)	(212	13)	(213	8)	(214	10)
(215	16)	(216	5)	(217	18)	(218	5)	(221	3)
(225	18)	(226	3)	(227	17)	(228	4)	(229	4)
(230	125)	(231	29)	(232	12)	(233	3)	(234	16)
(235	4)	(241	3)	(243	67)	(244	15)	(245	9)
(248	3)	(249	4)	(250	16)	(251	3)	(253	4)
(257	6)	(258	69)	(259	20)	(260	8)	(262	7)
(265	22)	(266	7)	(283	3)	(285	7)	(298	3)
(299	74)	(300	23)	(301	12)	(302	5)	(303	6)
(304	13)	(305	3)	(306	8)	(307	3)	(314	8)
(315	240)	(316	64)	(317	33)	(318	6)	(371	9)
(372	3)	(382	21)	(383	9)	(384	4)	(387	4)
(394	20)	(395	8)	(396	3)	(411	3)		

NAME:12C_2679.2_1160EC23_[837; alpha-D-Fructofuranose-1,6-bisphosphate (7TMS)]

210

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:268001-10-1

RI:2679

RT:16.787

NUM PEAKS: 170

(71	4)	(72	15)	(73	1000)	(74	88)	(75	110)
(76	6)	(77	9)	(81	8)	(82	21)	(83	7)
(85	5)	(86	3)	(87	4)	(89	5)	(96	13)
(97	7)	(98	4)	(99	6)	(100	3)	(101	15)
(102	6)	(103	33)	(104	4)	(105	3)	(109	8)
(111	5)	(113	12)	(115	8)	(116	5)	(117	21)
(118	3)	(119	6)	(125	5)	(127	6)	(128	3)
(129	86)	(130	14)	(131	20)	(133	53)	(134	7)
(135	13)	(137	4)	(140	13)	(141	17)	(142	11)
(143	24)	(144	6)	(145	5)	(146	3)	(147	199)
(148	32)	(149	29)	(150	3)	(151	9)	(153	3)
(155	9)	(156	8)	(157	17)	(158	4)	(159	3)
(163	3)	(167	3)	(169	12)	(177	9)	(181	7)
(182	3)	(183	11)	(184	4)	(187	3)	(189	10)
(190	7)	(191	37)	(192	6)	(193	10)	(195	10)
(196	5)	(197	4)	(199	3)	(200	14)	(201	4)
(202	3)	(203	3)	(204	37)	(205	17)	(206	5)
(207	25)	(208	5)	(209	5)	(210	3)	(211	49)
(212	8)	(213	6)	(214	11)	(215	57)	(216	14)
(217	63)	(218	14)	(219	8)	(221	33)	(222	9)
(223	5)	(225	29)	(226	6)	(227	16)	(228	3)
(229	9)	(230	68)	(231	23)	(232	7)	(241	6)
(243	10)	(244	3)	(255	5)	(257	36)	(258	9)
(259	5)	(269	3)	(270	4)	(271	15)	(272	4)
(273	3)	(281	7)	(283	8)	(284	3)	(285	9)
(295	10)	(296	3)	(297	3)	(298	7)	(299	124)
(300	34)	(301	18)	(302	3)	(303	7)	(305	3)
(313	5)	(314	7)	(315	166)	(316	46)	(317	24)
(318	5)	(319	7)	(328	22)	(329	7)	(330	3)
(341	3)	(343	6)	(345	4)	(347	6)	(348	3)
(355	3)	(356	4)	(357	10)	(358	3)	(361	3)
(369	7)	(370	3)	(371	3)	(373	7)	(387	17)
(388	7)	(389	4)	(423	3)	(436	3)	(444	5)
(445	24)	(446	11)	(447	6)	(513	3)	(589	6)

NAME:12C_2339.5_1160EC23_[882; Pseudouridine (5TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:234001-10-1

RI:2340

RT:14.991

NUM PEAKS: 133

(70	4)	(72	16)	(73	1000)	(74	79)	(75	31)
(82	3)	(86	4)	(89	8)	(98	1)	(99	6)
(100	30)	(101	13)	(103	86)	(104	6)	(105	3)
(106	5)	(111	5)	(113	6)	(115	2)	(116	3)
(117	12)	(119	4)	(122	1)	(125	5)	(126	1)
(127	17)	(128	1)	(129	35)	(130	3)	(131	24)
(132	3)	(133	47)	(134	5)	(135	2)	(136	1)
(140	3)	(141	2)	(142	7)	(143	30)	(144	5)
(145	3)	(147	159)	(148	24)	(149	17)	(151	2)
(154	3)	(157	6)	(158	6)	(159	1)	(166	2)
(172	2)	(177	2)	(179	1)	(180	1)	(184	1)
(185	2)	(186	2)	(189	13)	(191	7)	(192	3)
(193	2)	(198	2)	(201	2)	(202	5)	(203	3)
(204	5)	(207	2)	(209	2)	(211	1)	(215	26)

211

(216	7)	(217	498)	(218	97)	(219	44)	(220	4)
(221	2)	(225	2)	(229	1)	(230	18)	(231	3)
(239	4)	(252	1)	(253	5)	(254	2)	(255	4)
(257	3)	(265	2)	(266	1)	(267	10)	(268	2)
(269	25)	(270	6)	(281	4)	(282	2)	(283	7)
(285	1)	(327	2)	(329	1)	(355	13)	(356	9)
(357	64)	(358	22)	(359	10)	(369	3)	(370	3)
(371	9)	(372	5)	(373	2)	(382	2)	(383	9)
(384	5)	(385	2)	(386	4)	(409	2)	(410	1)
(411	10)	(412	5)	(423	5)	(424	32)	(425	18)
(426	8)	(443	1)	(496	6)	(497	5)	(498	2)
(499	3)	(500	2)	(501	2)	(513	1)	(514	3)
(589	5)	(590	2)	(591	2)				

NAME:12C_2651.1_1160EC15 [721; Adenosine (4TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:265001-10-1

RI:2651

RT:16.639

NUM PEAKS: 46

(73	1000)	(74	67)	(76	6)	(79	15)	(101	15)
(103	102)	(110	12)	(116	5)	(129	17)	(133	46)
(143	28)	(147	115)	(148	6)	(157	10)	(169	19)
(186	5)	(192	76)	(202	5)	(204	21)	(206	22)
(208	59)	(217	134)	(218	35)	(230	199)	(231	35)
(236	182)	(237	39)	(243	34)	(245	92)	(246	19)
(259	14)	(266	24)	(279	12)	(287	6)	(322	28)
(335	15)	(374	3)	(375	7)	(385	8)	(463	8)
(475	16)	(495	5)	(502	5)	(519	9)	(524	6)
(540	8)								

NAME:12C_1924.2_1313EC57_Mannitol (6TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:193002-10-1

RI:1924

RT:12.009

NUM PEAKS: 126

(70	2)	(72	14)	(73	1000)	(74	88)	(75	45)
(83	11)	(87	6)	(88	5)	(89	31)	(90	3)
(97	9)	(99	4)	(101	25)	(102	4)	(103	188)
(104	16)	(111	2)	(113	4)	(115	4)	(116	5)
(117	120)	(118	11)	(119	9)	(127	2)	(129	93)
(130	10)	(131	32)	(132	3)	(133	60)	(134	8)
(135	5)	(141	2)	(142	1)	(143	13)	(144	2)
(145	4)	(147	324)	(148	49)	(149	26)	(150	3)
(151	2)	(157	64)	(158	8)	(159	4)	(161	3)
(163	3)	(169	6)	(170	1)	(175	5)	(177	2)
(183	6)	(186	1)	(189	43)	(190	10)	(191	42)
(192	6)	(193	2)	(203	4)	(204	46)	(205	167)
(206	32)	(207	13)	(215	1)	(216	2)	(217	167)
(218	34)	(219	15)	(220	1)	(221	5)	(222	1)
(229	17)	(230	6)	(231	17)	(232	4)	(233	1)
(239	1)	(246	1)	(249	1)	(250	1)	(252	1)
(255	7)	(256	2)	(257	1)	(259	6)	(260	1)
(277	6)	(278	3)	(279	1)	(291	6)	(292	3)
(293	1)	(305	7)	(306	5)	(307	21)	(308	7)
(309	2)	(318	9)	(319	140)	(320	47)	(321	20)
(322	4)	(323	1)	(329	1)	(330	2)	(331	16)
(332	6)	(333	2)	(334	1)	(345	5)	(346	2)
(397	1)	(409	1)	(419	2)	(420	2)	(421	4)

212

(422 1) (423 1) (424 1) (433 1) (477 1)
 (485 1) (525 1) (526 1) (529 1) (552 1)
 (579 1)

NAME:12C 1920.1_1313EC57_1529; Methylcitric acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:192007-10-1

RI:1920

RT:11.983

NUM PEAKS: 157

(72 34) (73 1000) (74 107) (75 160) (76 8)
 (77 7) (80 2) (81 13) (83 4) (89 11)
 (90 3) (91 5) (92 2) (97 16) (99 8)
 (101 15) (104 7) (105 11) (109 8) (116 16)
 (118 7) (119 7) (122 2) (125 35) (127 6)
 (129 29) (131 41) (133 77) (134 11) (135 10)
 (136 3) (141 3) (143 12) (144 5) (145 4)
 (147 314) (148 50) (149 53) (150 6) (151 3)
 (152 2) (153 11) (155 22) (159 2) (161 3)
 (163 3) (169 12) (170 3) (171 16) (173 7)
 (181 5) (183 3) (185 3) (189 13) (190 6)
 (192 3) (193 2) (197 30) (198 4) (199 9)
 (203 6) (204 29) (207 7) (208 2) (209 3)
 (210 2) (215 4) (216 3) (218 18) (219 6)
 (221 19) (222 3) (225 5) (226 2) (227 3)
 (242 3) (243 50) (244 12) (245 11) (246 2)
 (247 1) (248 1) (249 2) (251 1) (252 2)
 (259 4) (271 7) (273 2) (278 2) (286 3)
 (287 106) (288 27) (289 11) (290 3) (291 3)
 (292 2) (293 2) (299 6) (300 1) (301 2)
 (305 4) (310 1) (314 1) (315 1) (325 3)
 (332 3) (333 3) (334 3) (335 1) (336 2)
 (337 1) (345 1) (347 3) (359 1) (360 4)
 (361 20) (362 6) (376 2) (377 10) (378 3)
 (386 2) (387 1) (388 1) (389 5) (403 1)
 (404 1) (408 1) (409 1) (410 1) (411 1)
 (414 2) (424 1) (429 1) (430 1) (439 2)
 (443 1) (449 1) (453 1) (456 1) (461 3)
 (477 1) (478 4) (479 7) (480 4) (481 3)
 (482 1) (485 1) (493 2) (496 2) (497 2)
 (508 1) (510 1) (526 2) (529 1) (547 1)
 (555 1) (558 1)

NAME:12C 1544.5_1313EC75_Erythronic acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:154001-10-1

RI:1545

RT:9.099

NUM PEAKS: 72

(70 335) (71 4) (72 13) (73 1000) (74 78)
 (83 10) (89 22) (99 5) (101 12) (102 92)
 (103 103) (104 12) (112 122) (113 11) (117 148)
 (118 12) (119 13) (129 35) (130 74) (131 35)
 (132 8) (133 70) (134 8) (135 6) (136 2)
 (139 2) (143 33) (144 9) (147 485) (148 79)
 (149 44) (150 5) (152 3) (163 5) (167 2)
 (177 17) (178 4) (180 6) (181 3) (185 3)
 (189 22) (190 3) (196 1) (203 7) (204 18)
 (205 100) (206 18) (214 35) (215 2) (217 84)
 (218 16) (219 12) (220 121) (229 10) (239 6)

213

(241	7)	(242	2)	(254	26)	(255	5)	(256	2)
(269	3)	(291	19)	(292	138)	(293	41)	(294	17)
(305	2)	(319	8)	(320	2)	(321	2)	(379	2)
(409	3)	(535	1)						

NAME:12C_1291.0_1185EK01_Leucine (2TMS)
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:129002-01-1
 RI:1291

NUM PEAKS: 98

(70	21)	(71	10)	(72	27)	(73	1000)	(74	112)
(75	178)	(76	14)	(77	55)	(78	5)	(79	8)
(80	2)	(81	1)	(82	4)	(83	3)	(84	13)
(85	7)	(86	46)	(87	10)	(88	4)	(89	4)
(90	1)	(91	1)	(92	2)	(93	1)	(94	1)
(95	1)	(96	5)	(97	3)	(98	6)	(99	10)
(100	89)	(101	17)	(102	168)	(103	44)	(104	9)
(105	5)	(110	1)	(111	1)	(112	3)	(113	2)
(114	4)	(115	25)	(116	32)	(117	25)	(118	5)
(119	5)	(126	2)	(127	1)	(128	23)	(129	9)
(130	41)	(131	19)	(132	20)	(133	41)	(134	7)
(135	3)	(140	1)	(142	14)	(143	4)	(144	5)
(145	1)	(146	4)	(147	117)	(148	19)	(149	10)
(150	1)	(156	3)	(157	2)	(158	720)	(159	105)
(160	32)	(161	3)	(163	1)	(170	8)	(171	2)
(172	1)	(174	3)	(175	2)	(176	2)	(177	2)
(186	1)	(188	1)	(191	1)	(202	1)	(203	3)
(204	2)	(205	4)	(206	1)	(207	1)	(218	21)
(219	5)	(220	2)	(231	1)	(232	25)	(233	6)
(234	2)	(260	7)	(261	2)				

NAME:12C_1273.1_1313EC43_[938; Sulfuric acid (2TMS)]
 COMMENTS:Kopka J, MPIMP, Dept. Willmitzer
 CASNO:127005-10-1
 RI:1273

RT:6.066

NUM PEAKS: 344

(72	37)	(73	278)	(74	26)	(76	10)	(83	5)
(84	13)	(88	7)	(89	23)	(90	7)	(94	4)
(95	11)	(98	7)	(107	12)	(108	9)	(109	7)
(111	6)	(112	6)	(113	5)	(114	15)	(115	17)
(116	16)	(118	12)	(119	13)	(120	9)	(122	9)
(123	18)	(125	12)	(128	6)	(130	4)	(132	30)
(133	33)	(134	18)	(137	5)	(138	10)	(139	28)
(140	8)	(141	10)	(143	7)	(144	4)	(145	9)
(147	1000)	(148	179)	(149	106)	(150	17)	(151	7)
(152	7)	(153	6)	(154	8)	(155	4)	(156	6)
(158	7)	(159	9)	(160	6)	(162	10)	(164	4)
(165	5)	(168	9)	(169	7)	(170	6)	(171	6)
(172	5)	(173	5)	(177	6)	(181	7)	(182	8)
(184	7)	(185	5)	(186	9)	(187	7)	(188	7)
(189	6)	(190	6)	(191	7)	(193	3)	(194	4)
(197	8)	(198	7)	(201	5)	(202	6)	(205	8)
(206	3)	(208	6)	(209	6)	(210	6)	(211	8)
(216	6)	(217	8)	(218	6)	(222	5)	(223	6)
(224	4)	(226	7)	(227	187)	(228	32)	(229	28)
(230	11)	(233	4)	(234	2)	(235	5)	(236	8)
(237	7)	(238	6)	(239	6)	(240	7)	(241	6)
(242	7)	(243	8)	(244	6)	(245	8)	(247	8)
(249	6)	(250	6)	(252	8)	(253	7)	(254	9)

214

(255	8)	(256	8)	(257	4)	(258	8)	(262	7)
(263	7)	(264	4)	(265	8)	(267	9)	(270	8)
(271	9)	(272	9)	(275	9)	(277	11)	(279	12)
(280	12)	(281	9)	(282	10)	(283	8)	(284	7)
(288	9)	(289	7)	(292	7)	(293	8)	(296	5)
(297	8)	(300	9)	(301	6)	(302	10)	(303	3)
(306	4)	(308	3)	(309	4)	(310	5)	(311	4)
(313	5)	(314	4)	(316	8)	(317	6)	(319	5)
(320	4)	(322	7)	(325	6)	(326	9)	(327	6)
(328	10)	(329	8)	(330	9)	(331	7)	(332	7)
(333	8)	(334	5)	(335	6)	(336	6)	(338	5)
(341	6)	(342	7)	(345	6)	(346	7)	(347	8)
(348	7)	(349	7)	(350	6)	(351	9)	(352	6)
(353	9)	(354	12)	(355	6)	(356	9)	(358	11)
(360	4)	(361	7)	(362	8)	(363	13)	(369	12)
(373	8)	(374	8)	(375	15)	(376	8)	(381	9)
(382	7)	(383	7)	(384	11)	(385	10)	(386	12)
(388	10)	(389	12)	(393	6)	(394	6)	(395	9)
(396	16)	(398	7)	(400	11)	(401	10)	(402	9)
(403	8)	(406	8)	(407	9)	(408	8)	(409	7)
(410	7)	(411	4)	(415	7)	(416	8)	(417	8)
(418	7)	(419	5)	(420	7)	(421	6)	(422	7)
(423	4)	(424	6)	(425	10)	(426	4)	(428	5)
(429	7)	(430	10)	(431	8)	(432	4)	(433	4)
(435	5)	(436	7)	(439	6)	(440	6)	(441	10)
(442	7)	(443	5)	(444	5)	(445	7)	(446	6)
(449	8)	(452	9)	(453	10)	(454	8)	(457	4)
(458	7)	(459	10)	(460	11)	(462	8)	(463	10)
(465	10)	(466	12)	(467	7)	(468	9)	(469	8)
(470	11)	(471	8)	(472	6)	(474	8)	(475	6)
(476	7)	(477	10)	(478	9)	(479	6)	(481	9)
(482	11)	(483	5)	(484	6)	(485	8)	(486	14)
(487	9)	(488	7)	(489	5)	(492	8)	(494	10)
(495	7)	(496	11)	(498	8)	(499	11)	(500	11)
(502	11)	(503	10)	(505	6)	(506	12)	(509	4)
(510	6)	(511	6)	(512	8)	(513	8)	(514	5)
(516	7)	(517	12)	(518	8)	(519	5)	(521	7)
(522	9)	(523	5)	(524	7)	(525	5)	(526	9)
(528	9)	(529	12)	(530	6)	(531	7)	(532	7)
(533	7)	(534	7)	(535	9)	(536	4)	(537	11)
(538	8)	(539	4)	(541	7)	(545	6)	(546	4)
(548	9)	(549	8)	(551	5)	(552	7)	(553	2)
(555	5)	(556	3)	(557	4)	(558	7)	(559	4)
(561	6)	(563	3)	(564	4)	(565	4)	(567	3)
(570	5)	(572	6)	(573	4)	(578	4)	(579	4)
(580	3)	(583	3)	(589	5)	(595	2)		

NAME:12C_1269.8_1135EC44_Urea (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:127002-01-1

RI:1270

RT:402.296

RSN:2975.0

NUM PEAKS: 51

(70	62)	(71	56)	(72	79)	(73	377)	(74	147)
(75	115)	(76	11)	(77	6)	(78	21)	(79	64)
(80	5)	(84	10)	(85	24)	(86	21)	(87	78)
(88	10)	(90	6)	(99	136)	(100	100)	(101	33)
(102	20)	(103	12)	(105	8)	(111	5)	(113	15)
(114	15)	(115	31)	(116	12)	(117	6)	(130	68)

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(131 67) (132 56) (133 31) (134 6) (146 66)
 (147 1000) (148 161) (149 78) (150 7) (155 4)
 (157 15) (171 158) (172 29) (173 65) (174 11)
 (175 4) (186 9) (189 434) (190 79) (191 35)
 (204 21)

NAME:12C 1723.7 1160EC15 2-Aminoadipic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:172006-10-1

RI:1724

RT:10.996

NUM PEAKS: 183

(70 20) (71 15) (72 35) (73 1000) (74 100)
 (75 283) (76 21) (77 23) (78 5) (79 9)
 (80 12) (81 8) (82 6) (83 11) (85 28)
 (86 15) (87 9) (88 5) (89 6) (91 2)
 (92 1) (93 15) (94 2) (95 9) (96 8)
 (97 20) (98 47) (99 17) (100 135) (101 24)
 (102 12) (104 5) (107 2) (108 10) (109 3)
 (110 3) (111 9) (112 9) (113 4) (114 13)
 (115 86) (116 30) (117 29) (118 5) (119 7)
 (121 1) (122 1) (123 4) (124 2) (125 2)
 (126 5) (127 4) (128 219) (129 199) (130 36)
 (131 53) (132 23) (133 58) (134 9) (135 6)
 (136 1) (137 3) (138 3) (141 2) (142 8)
 (143 7) (144 2) (145 6) (146 3) (147 178)
 (148 31) (149 39) (150 6) (151 14) (152 4)
 (153 4) (154 33) (159 3) (161 2) (162 1)
 (163 12) (164 3) (165 1) (168 3) (169 1)
 (170 37) (171 6) (172 13) (174 10) (175 2)
 (182 13) (183 3) (187 1) (188 11) (193 2)
 (198 1) (200 2) (202 8) (203 18) (208 1)
 (213 2) (216 4) (217 304) (218 87) (219 34)
 (220 5) (221 6) (228 8) (231 1) (232 2)
 (233 2) (234 1) (235 1) (242 2) (243 11)
 (244 71) (245 18) (246 8) (250 1) (251 1)
 (252 1) (254 2) (256 1) (259 3) (260 357)
 (261 83) (262 33) (263 5) (266 1) (272 28)
 (273 6) (274 3) (278 1) (286 1) (287 1)
 (288 6) (289 2) (290 1) (291 7) (292 2)
 (293 2) (294 1) (301 2) (302 2) (313 1)
 (317 1) (318 1) (326 1) (334 3) (335 2)
 (337 1) (342 1) (348 1) (361 1) (362 15)
 (363 6) (364 3) (376 1) (377 9) (378 4)
 (379 1) (391 1) (393 1) (417 1) (418 2)
 (428 1) (438 1) (450 1) (465 1) (472 1)
 (478 1) (486 1) (497 1) (503 1) (513 1)
 (523 1) (529 1) (532 1) (537 1) (540 1)
 (541 1) (547 1) (562 1)

NAME:12C 1739.1 1274EC11 Aspartic acid (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:174003-10-1

RI:1739

RT:11.121

NUM PEAKS: 117

(70 40) (71 24) (72 30) (73 1000) (74 102)
 (79 20) (80 14) (88 6) (89 30) (92 5)
 (94 9) (96 9) (98 9) (99 46) (100 58)
 (105 24) (106 9) (107 5) (108 4) (113 7)

216

(114	10)	(121	4)	(124	5)	(127	21)	(130	26)
(131	23)	(133	89)	(134	11)	(135	5)	(141	13)
(142	8)	(143	22)	(144	6)	(145	4)	(146	13)
(149	25)	(150	10)	(157	22)	(158	19)	(159	36)
(160	11)	(161	8)	(162	3)	(163	83)	(164	17)
(169	12)	(171	16)	(172	75)	(173	25)	(177	7)
(183	10)	(185	18)	(188	6)	(191	26)	(197	4)
(199	10)	(202	33)	(205	243)	(206	45)	(207	23)
(213	6)	(215	34)	(216	13)	(221	26)	(222	9)
(223	7)	(242	4)	(244	8)	(246	6)	(247	6)
(257	5)	(259	6)	(262	5)	(264	4)	(273	26)
(275	9)	(276	5)	(279	21)	(280	9)	(287	12)
(288	21)	(289	22)	(290	24)	(291	8)	(299	8)
(302	5)	(304	31)	(306	7)	(316	5)	(317	7)
(330	7)	(331	13)	(332	6)	(347	8)	(363	14)
(364	7)	(365	5)	(378	8)	(379	5)	(380	6)
(382	3)	(406	14)	(407	10)	(421	3)	(422	5)
(424	7)	(430	5)	(432	5)	(454	6)	(498	7)
(506	4)	(511	5)	(519	4)	(527	4)	(529	4)
(553	4)	(565	4)						

NAME:12C 2225.6_1178EC20_Tryptophan (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:223001-10-1

RI:2226

RT:14.362

NUM PEAKS: 95

(72	12)	(73	1000)	(76	6)	(77	12)	(91	3)
(92	3)	(94	3)	(96	25)	(100	13)	(103	3)
(105	8)	(106	3)	(110	8)	(116	15)	(122	3)
(124	3)	(128	7)	(129	32)	(130	19)	(131	41)
(132	42)	(133	21)	(134	8)	(138	3)	(142	3)
(145	48)	(146	17)	(147	29)	(148	5)	(152	7)
(155	3)	(156	9)	(159	9)	(160	8)	(161	6)
(170	3)	(173	5)	(175	3)	(180	8)	(184	6)
(187	12)	(188	8)	(189	7)	(190	8)	(200	11)
(201	5)	(202	705)	(203	155)	(204	45)	(215	8)
(218	17)	(219	30)	(220	10)	(221	5)	(222	5)
(229	3)	(230	8)	(231	7)	(232	3)	(233	4)
(235	7)	(236	3)	(246	3)	(248	3)	(257	3)
(261	4)	(264	6)	(265	6)	(291	38)	(292	15)
(293	6)	(303	4)	(327	4)	(337	4)	(338	4)
(351	4)	(367	3)	(379	3)	(394	3)	(406	4)
(407	8)	(408	9)	(409	3)	(421	3)	(422	10)
(423	8)	(424	4)	(425	3)	(427	3)	(437	4)
(446	3)	(462	5)	(496	3)	(542	3)	(564	3)

NAME:12C 2770.4_1160EC15_[626; 5'-Methylthioadenosine (3TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:277004-10-1

RI:2770

RT:17.269

NUM PEAKS: 24

(73	1000)	(74	105)	(87	43)	(101	75)	(108	46)
(115	35)	(116	53)	(119	32)	(127	34)	(135	63)
(136	276)	(137	30)	(148	36)	(164	692)	(165	43)
(169	261)	(175	769)	(176	98)	(177	35)	(188	441)
(190	35)	(208	45)	(234	13)	(426	28)		

NAME:12C_1324.1_1313EC07_Nicotinic acid (1TMS)

217

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:133004-10-1

RI:1324

RT:6.689

NUM PEAKS: 17

(78	769)	(79	88)	(83	111)	(106	622)	(107	47)
(110	11)	(111	38)	(112	48)	(136	836)	(137	90)
(138	26)	(141	49)	(180	1000)	(181	149)	(182	36)
(186	61)	(195	41)						

NAME:12C_2427.5_1313EC07_[931; myo-Inositol-1-phosphate (7TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:243001-10-1

RI:2428

RT:14.977

NUM PEAKS: 283

(70	3)	(71	3)	(72	16)	(73	1000)	(74	89)
(75	76)	(76	4)	(77	10)	(78	1)	(79	3)
(80	1)	(81	14)	(82	2)	(83	4)	(84	1)
(85	5)	(86	2)	(87	6)	(88	2)	(89	5)
(90	1)	(91	3)	(92	1)	(93	2)	(94	1)
(95	2)	(96	2)	(97	2)	(98	2)	(99	5)
(100	1)	(101	8)	(102	4)	(103	25)	(105	6)
(106	2)	(107	3)	(108	1)	(109	5)	(110	1)
(111	6)	(112	1)	(113	5)	(114	1)	(115	7)
(116	5)	(117	7)	(118	1)	(119	6)	(120	1)
(121	3)	(123	1)	(125	2)	(126	1)	(127	6)
(128	1)	(129	36)	(130	4)	(131	21)	(132	4)
(133	64)	(134	9)	(135	13)	(136	2)	(137	6)
(138	1)	(139	2)	(140	1)	(141	3)	(142	3)
(143	18)	(144	2)	(145	3)	(146	1)	(147	252)
(148	41)	(149	26)	(150	3)	(151	6)	(152	1)
(153	5)	(154	2)	(155	5)	(156	4)	(157	5)
(158	1)	(159	2)	(160	1)	(161	3)	(162	1)
(163	3)	(164	1)	(165	2)	(166	1)	(167	2)
(168	1)	(169	5)	(170	1)	(171	1)	(173	1)
(175	3)	(176	1)	(177	3)	(178	1)	(179	2)
(180	1)	(181	8)	(182	2)	(183	4)	(184	1)
(185	1)	(187	1)	(189	8)	(190	7)	(191	47)
(192	9)	(193	12)	(194	2)	(195	4)	(196	1)
(197	2)	(199	1)	(201	2)	(202	1)	(203	2)
(204	15)	(205	7)	(206	2)	(207	15)	(208	4)
(209	3)	(210	2)	(211	35)	(212	6)	(213	4)
(214	1)	(215	4)	(216	2)	(217	46)	(218	10)
(219	4)	(221	8)	(222	2)	(223	1)	(224	1)
(225	9)	(226	2)	(227	11)	(228	3)	(229	2)
(230	11)	(231	4)	(232	1)	(233	1)	(235	1)
(237	1)	(239	2)	(240	1)	(241	2)	(242	1)
(243	11)	(244	3)	(245	3)	(246	9)	(247	2)
(248	1)	(249	1)	(251	1)	(252	1)	(253	1)
(254	1)	(255	8)	(256	2)	(257	3)	(258	1)
(259	1)	(265	3)	(266	1)	(267	1)	(268	1)
(269	3)	(270	2)	(271	3)	(272	1)	(273	1)
(278	1)	(283	4)	(284	2)	(285	7)	(286	2)
(287	1)	(291	5)	(292	2)	(293	1)	(297	1)
(298	12)	(299	108)	(300	32)	(301	17)	(302	3)
(303	1)	(304	2)	(305	8)	(306	4)	(307	2)
(308	1)	(312	1)	(313	4)	(314	11)	(315	89)
(316	26)	(317	25)	(318	104)	(319	35)	(320	15)
(321	3)	(322	1)	(327	1)	(328	1)	(329	1)

218

(330	1)	(331	2)	(332	1)	(333	1)	(340	1)
(341	2)	(342	3)	(343	8)	(344	4)	(345	5)
(346	2)	(347	1)	(357	1)	(358	1)	(359	1)
(360	1)	(367	1)	(368	1)	(369	1)	(370	1)
(371	1)	(372	2)	(373	6)	(374	3)	(375	1)
(385	2)	(386	11)	(387	39)	(388	19)	(389	19)
(390	6)	(391	3)	(392	1)	(417	1)	(418	1)
(419	2)	(420	1)	(421	1)	(428	1)	(429	3)
(430	1)	(431	2)	(432	5)	(433	4)	(434	2)
(435	1)	(441	1)	(442	1)	(443	1)	(444	1)
(455	1)	(456	1)	(457	1)	(458	1)	(459	1)
(460	1)	(461	1)	(462	1)	(469	1)	(470	2)
(471	1)	(472	1)	(507	1)				

NAME:12C_2000.0_1313EC07_Panthotenic acid (3TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:200006-10-1

RI:2000

RT:12.490

NUM PEAKS: 107

(78	209)	(79	192)	(80	14)	(108	92)	(109	16)
(123	74)	(124	132)	(127	69)	(128	70)	(129	254)
(143	25)	(157	1000)	(166	33)	(170	38)	(182	1)
(184	30)	(185	15)	(197	4)	(198	16)	(201	777)
(202	71)	(247	119)	(274	8)	(284	7)	(285	26)
(286	9)	(290	82)	(291	871)	(292	113)	(330	17)
(346	72)	(347	28)	(359	43)	(360	3)	(361	18)
(374	21)	(375	21)	(386	18)	(390	14)	(391	15)
(406	68)	(420	168)	(421	85)	(433	7)	(434	44)
(445	66)	(446	27)	(448	20)	(449	1)	(450	5)
(463	50)	(465	16)	(467	4)	(468	5)	(475	3)
(480	18)	(481	13)	(482	53)	(487	55)	(493	34)
(494	12)	(496	29)	(497	17)	(502	9)	(505	28)
(506	19)	(510	5)	(511	55)	(514	35)	(515	15)
(516	7)	(519	67)	(522	73)	(523	12)	(524	49)
(525	1)	(526	3)	(534	60)	(539	64)	(540	13)
(543	76)	(545	5)	(547	57)	(548	15)	(549	20)
(551	20)	(552	68)	(553	1)	(557	14)	(562	4)
(563	6)	(569	8)	(570	37)	(575	6)	(577	26)
(579	13)	(580	16)	(582	12)	(583	25)	(585	13)
(586	14)	(588	28)	(591	12)	(593	12)	(595	10)
(596	14)	(597	2)						

NAME:12C_1292.9_1313EC11_Leucine (2TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:129002-10-1

RI:1293

RT:6.287

NUM PEAKS: 4

(79	83)	(158	1000)	(159	20)	(232	2)
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NAME:12C_1490.1_2119DC04_[545; 2,3-Dimethylsuccinic acid (2TMS)]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:149003-10-1

RI:1490

RT:20.245

NUM PEAKS: 166

(41	217)	(42	21)	(43	227)	(44	61)	(45	122)
(47	52)	(50	20)	(52	23)	(53	34)	(54	11)
(57	15)	(58	41)	(59	316)	(60	26)	(61	65)

219

(62	6)	(63	11)	(65	17)	(66	6)	(67	79)
(68	21)	(69	185)	(70	11)	(71	52)	(72	11)
(73	408)	(74	32)	(75	1000)	(76	82)	(77	49)
(79	35)	(81	30)	(82	19)	(83	116)	(84	6)
(85	123)	(86	13)	(89	734)	(90	61)	(91	64)
(92	7)	(93	8)	(95	128)	(96	18)	(97	46)
(98	10)	(99	55)	(103	19)	(105	44)	(107	8)
(108	2)	(110	4)	(111	9)	(113	267)	(114	22)
(119	9)	(120	4)	(123	15)	(125	17)	(127	72)
(131	84)	(132	11)	(137	7)	(139	2)	(141	20)
(143	479)	(144	55)	(145	114)	(146	42)	(147	826)
(148	134)	(149	30)	(154	5)	(155	79)	(156	11)
(157	278)	(158	38)	(159	237)	(160	27)	(161	85)
(162	24)	(163	355)	(164	53)	(165	34)	(166	7)
(169	8)	(170	18)	(173	41)	(174	13)	(179	3)
(180	6)	(185	31)	(186	8)	(187	44)	(191	310)
(192	43)	(193	30)	(196	4)	(197	3)	(201	59)
(207	435)	(208	64)	(209	47)	(210	7)	(212	2)
(213	5)	(215	14)	(216	7)	(217	12)	(226	3)
(229	72)	(231	184)	(232	33)	(239	2)	(244	2)
(247	174)	(248	36)	(249	20)	(250	5)	(254	5)
(258	3)	(259	28)	(261	24)	(262	3)	(270	3)
(271	3)	(275	362)	(276	92)	(277	35)	(278	5)
(291	87)	(292	21)	(293	7)	(299	4)	(301	2)
(313	3)	(319	46)	(320	10)	(321	2)	(322	2)
(333	3)	(346	2)	(354	2)	(356	2)	(371	2)
(380	3)	(388	2)	(397	2)	(407	3)	(434	2)
(439	3)	(453	2)	(466	3)	(476	2)	(479	3)
(515	2)	(521	2)	(527	2)	(533	2)	(552	2)
(562	3)	(567	2)	(579	2)	(594	2)	(596	5)
(598	7)								

NAME:12C_2816.0_2119DC04_[542; Maltose methoxyamine {BP} (8TMS); alpha-D-Glc-(1,4)-alpha-D-Glc]

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer

CASNO:282003-10-1

RI:2816

RT:41.182

NUM PEAKS: 75

(44	171)	(48	62)	(64	42)	(73	1000)	(82	73)
(88	62)	(103	130)	(104	92)	(108	67)	(111	127)
(129	273)	(130	78)	(133	147)	(143	44)	(147	245)
(152	34)	(167	53)	(169	195)	(172	33)	(175	40)
(179	127)	(181	52)	(191	520)	(192	167)	(197	50)
(202	43)	(207	109)	(214	26)	(215	29)	(217	105)
(218	44)	(220	30)	(229	57)	(236	29)	(241	39)
(242	28)	(243	110)	(244	76)	(246	29)	(251	35)
(252	59)	(267	42)	(270	47)	(275	32)	(281	53)
(319	64)	(321	44)	(323	32)	(333	45)	(353	24)
(357	55)	(361	166)	(362	69)	(363	56)	(386	29)
(393	25)	(400	22)	(407	40)	(431	37)	(439	27)
(443	24)	(457	24)	(464	36)	(469	41)	(488	29)
(506	37)	(507	25)	(509	37)	(521	27)	(523	25)
(530	33)	(550	24)	(581	26)	(587	26)	(597	24)

NAME:12C_1685.1_1313EC57_Ribose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685

CASNO:168002-10-1

RI:1685

RT:10.186

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SOURCE: C:\NISTMS\AMDIS32\LIB\MS_RI.msp

NUM PEAKS: 431

(70	75)	(71	28)	(73	1000)	(74	24)	(78	10)
(82	16)	(83	39)	(84	24)	(85	16)	(86	7)
(87	13)	(88	10)	(89	66)	(90	11)	(91	28)
(92	6)	(95	5)	(96	4)	(97	4)	(98	8)
(99	17)	(101	33)	(102	5)	(103	282)	(104	31)
(105	37)	(106	6)	(107	4)	(108	2)	(109	21)
(111	5)	(112	10)	(113	17)	(117	59)	(119	18)
(120	5)	(121	5)	(122	4)	(123	4)	(126	9)
(127	8)	(128	18)	(129	43)	(133	69)	(135	8)
(136	2)	(137	6)	(138	5)	(139	5)	(140	15)
(143	6)	(144	40)	(145	19)	(147	244)	(148	42)
(149	17)	(151	6)	(152	4)	(153	4)	(155	55)
(156	12)	(157	8)	(158	10)	(160	127)	(161	23)
(162	11)	(163	11)	(164	6)	(165	4)	(166	3)
(167	7)	(168	6)	(170	7)	(171	4)	(172	7)
(173	27)	(174	19)	(175	12)	(176	5)	(177	6)
(178	5)	(179	3)	(181	5)	(182	7)	(183	5)
(184	7)	(186	6)	(187	7)	(189	44)	(190	17)
(191	17)	(192	6)	(194	6)	(195	7)	(196	5)
(197	6)	(198	6)	(199	12)	(200	18)	(201	9)
(203	8)	(204	16)	(205	34)	(206	12)	(207	5)
(208	4)	(209	5)	(210	3)	(212	4)	(213	11)
(216	8)	(217	133)	(218	30)	(219	16)	(221	6)
(222	5)	(223	5)	(224	3)	(225	3)	(228	4)
(229	5)	(230	8)	(233	19)	(234	8)	(235	5)
(236	3)	(237	4)	(239	2)	(240	6)	(241	2)
(242	6)	(245	12)	(246	7)	(247	5)	(248	6)
(249	3)	(250	6)	(251	5)	(252	4)	(254	6)
(255	4)	(256	6)	(257	7)	(260	3)	(261	4)
(262	9)	(263	15)	(264	8)	(265	6)	(266	5)
(267	4)	(268	6)	(269	5)	(270	5)	(271	6)
(272	5)	(273	4)	(274	5)	(276	6)	(277	14)
(278	6)	(279	6)	(280	3)	(281	5)	(282	5)
(283	3)	(284	4)	(285	3)	(286	6)	(287	10)
(289	5)	(290	31)	(291	15)	(292	8)	(293	6)
(294	5)	(295	5)	(296	5)	(297	5)	(298	4)
(299	7)	(300	5)	(302	7)	(303	3)	(304	2)
(306	3)	(307	42)	(308	15)	(309	9)	(310	6)
(311	4)	(313	3)	(314	3)	(315	2)	(317	3)
(318	4)	(319	6)	(322	3)	(323	3)	(324	4)
(325	4)	(326	4)	(327	5)	(328	3)	(329	2)
(330	3)	(331	4)	(332	6)	(335	5)	(336	4)
(337	5)	(338	5)	(339	4)	(342	3)	(343	2)
(344	2)	(345	2)	(346	3)	(347	4)	(349	4)
(350	2)	(351	4)	(352	7)	(353	5)	(354	3)
(355	2)	(357	3)	(358	5)	(359	4)	(360	5)
(361	3)	(362	5)	(363	2)	(364	6)	(365	7)
(366	6)	(367	6)	(368	4)	(370	3)	(371	3)
(372	5)	(373	5)	(374	4)	(375	2)	(377	4)
(379	3)	(380	4)	(381	6)	(382	4)	(383	4)
(384	3)	(385	3)	(386	3)	(387	5)	(388	4)
(389	3)	(390	5)	(391	4)	(392	3)	(393	4)
(394	3)	(395	3)	(396	4)	(397	4)	(399	4)
(401	3)	(402	5)	(403	4)	(404	5)	(405	3)
(406	4)	(407	5)	(408	2)	(411	7)	(412	5)
(413	5)	(414	5)	(415	4)	(416	4)	(419	4)
(420	6)	(421	4)	(422	2)	(423	2)	(424	4)
(425	4)	(426	6)	(427	3)	(428	5)	(429	6)

221

(430	4)	(431	2)	(432	2)	(434	5)	(435	4)
(436	6)	(437	3)	(439	3)	(440	4)	(442	2)
(443	5)	(444	5)	(445	5)	(446	4)	(447	3)
(448	5)	(449	6)	(450	3)	(451	3)	(452	5)
(453	4)	(454	2)	(455	4)	(456	4)	(457	6)
(458	5)	(459	3)	(460	3)	(461	2)	(462	6)
(463	3)	(465	3)	(466	3)	(467	5)	(468	5)
(469	5)	(470	4)	(471	2)	(474	3)	(475	2)
(477	2)	(478	4)	(479	3)	(480	3)	(481	4)
(482	4)	(483	2)	(484	4)	(485	3)	(486	3)
(487	3)	(489	3)	(490	4)	(491	5)	(492	2)
(493	4)	(494	4)	(496	3)	(497	5)	(498	4)
(499	3)	(500	3)	(501	5)	(502	3)	(503	4)
(504	4)	(505	5)	(506	4)	(507	2)	(509	5)
(510	3)	(511	4)	(512	7)	(513	4)	(514	2)
(515	6)	(516	5)	(517	4)	(518	4)	(519	5)
(520	3)	(521	3)	(523	4)	(524	5)	(525	4)
(526	5)	(527	4)	(528	2)	(529	3)	(530	6)
(531	5)	(532	6)	(533	3)	(534	5)	(536	3)
(537	3)	(538	2)	(539	4)	(540	4)	(541	4)
(542	3)	(543	6)	(544	5)	(545	5)	(546	3)
(547	4)	(548	3)	(549	3)	(550	5)	(551	4)
(552	2)	(553	2)	(555	3)	(556	1)	(557	2)
(558	3)	(559	3)	(560	2)	(561	3)	(562	3)
(563	2)	(564	3)	(565	2)	(566	2)	(567	3)
(569	3)	(570	2)	(571	2)	(572	5)	(574	2)
(575	3)	(577	1)	(578	1)	(579	1)	(580	1)
(582	1)	(583	1)	(588	1)	(590	2)	(592	1)
(593	1)								

NAME:13C 1685.1 1313EC16_Ribose methoxyamine (4TMS)

COMMENTS:Kopka J, MPIMP, Dept. Willmitzer |RI:1685 |RI:1685 |RI:1685

CASNO:168002-11-1

RI:1685

RT:10.202

SOURCE:C:\NISTMS\AMDIS32\LIB\MS_RI.msp

NUM PEAKS: 272

(70	9)	(71	18)	(72	34)	(73	1000)	(74	136)
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(87	16)	(88	12)	(89	29)	(90	11)	(91	26)
(92	5)	(95	1)	(96	1)	(98	1)	(99	6)
(100	14)	(101	47)	(102	38)	(103	31)	(104	202)
(105	32)	(106	8)	(108	1)	(109	1)	(113	2)
(114	2)	(115	9)	(116	20)	(117	32)	(118	141)
(119	50)	(120	10)	(121	3)	(122	2)	(127	1)
(128	5)	(129	2)	(130	10)	(131	37)	(132	55)
(133	81)	(134	76)	(135	13)	(136	3)	(138	3)
(139	1)	(141	2)	(142	2)	(143	4)	(144	58)
(145	13)	(146	17)	(147	186)	(148	32)	(149	21)
(150	4)	(151	2)	(153	2)	(156	1)	(157	2)
(158	6)	(159	2)	(160	5)	(161	8)	(162	41)
(163	12)	(164	3)	(165	1)	(167	1)	(168	1)
(169	1)	(172	3)	(173	10)	(174	6)	(175	6)
(176	8)	(177	7)	(178	1)	(179	2)	(181	2)
(187	1)	(188	3)	(189	37)	(190	15)	(191	37)
(192	13)	(193	2)	(194	2)	(196	1)	(197	1)
(201	3)	(202	2)	(203	7)	(204	14)	(205	6)
(206	16)	(207	12)	(208	3)	(209	1)	(211	3)
(212	1)	(216	3)	(217	5)	(218	9)	(219	10)

(220	114)	(221	21)	(222	10)	(224	1)	(225	3)
(226	1)	(230	1)	(232	6)	(233	5)	(234	52)
(235	20)	(236	7)	(237	3)	(238	2)	(239	1)
(245	2)	(247	5)	(248	5)	(252	1)	(255	1)
(257	3)	(259	1)	(261	2)	(262	10)	(263	3)
(264	2)	(265	3)	(266	2)	(267	3)	(268	3)
(269	1)	(270	1)	(271	3)	(272	1)	(274	1)
(276	1)	(278	5)	(279	9)	(280	5)	(281	1)
(283	2)	(285	1)	(286	2)	(287	1)	(293	3)
(294	4)	(295	1)	(297	1)	(298	2)	(299	1)
(302	2)	(303	1)	(304	1)	(307	2)	(308	2)
(309	3)	(310	31)	(311	8)	(312	3)	(313	1)
(314	1)	(315	2)	(316	1)	(317	1)	(320	1)
(324	2)	(325	1)	(326	1)	(327	1)	(333	1)
(334	1)	(337	2)	(338	1)	(341	1)	(342	1)
(346	1)	(348	1)	(351	1)	(352	2)	(353	1)
(357	1)	(360	1)	(361	1)	(362	1)	(363	1)
(368	2)	(369	3)	(370	2)	(372	1)	(373	1)
(377	1)	(380	1)	(385	1)	(386	2)	(387	1)
(390	1)	(393	1)	(394	2)	(395	1)	(401	1)
(407	1)	(416	1)	(418	2)	(419	1)	(421	1)
(425	1)	(426	1)	(427	2)	(428	2)	(435	2)
(436	1)	(439	2)	(443	1)	(446	1)	(447	1)
(450	2)	(451	4)	(452	1)	(453	2)	(454	2)
(455	1)	(462	2)	(463	1)	(466	1)	(467	2)
(471	1)	(479	2)	(483	1)	(487	1)	(492	1)
(494	2)	(508	1)	(509	1)	(510	2)	(511	1)
(513	2)	(516	1)	(523	2)	(525	1)	(528	1)
(529	1)	(530	1)	(531	2)	(537	1)	(538	2)
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223

Table 4

1102.5_1185EK02	999	446	223	312	294	652	348	195	355	191
283	377	360	448	349	367	306	270	366	402	411
341	242	387	462	253	365	386	326	417	388	386
417	410	329	358	344	205	361	511	353	347	267
271	348	365	275	232	302	324	298	330	333	343
315	278	307	290	323	549	284	223	291	249	363
258	319	352	364	211	264	299	377	289	245	312
294	308	341	250	340	312	210	287	318	277	276
287	300	288	312	294	227	309	315	318	272	284
280	296	285	179	291	197	291	291	355	298	294
227	257	258	270	321	256	295	302	219	303	260
237	237	205	276	260	256	220	267	363	325	254
205	317	264	233	330	324	194	328	306	337	170
231	371	246	256	252	253	264	287	276	318	276
252	257	260	295	279	265	289	245	276	254	278
247	187	236	241	311	292	215	248	167	255	252
228	232	243	241	192	202	261	253	232	180	288
371	353	132	227	645	348	390	136	203	420	168
325	339	354	248	267	317	312	384	372	205	495
582	237	448	487	340	330	378	346	311	226	342
267	350	223	238	344	273	272	258	338	292	203
239	0	257	195	332	282	322	306	322	354	51
257	129	552	334	277	322	159	307	332	315	359
164	263	204	341	253	336	287	87	234	326	265
189	326	329	257	221	300	284	284	191	119	324
179	298	292	248	337	208	272	189	287	179	266
0	227	145	270	333	332	281	190	287	317	319
259	287	343	296	258	288	259	261	324	313	256
244	27	283	294	260	376	209	354	337	287	301
230	250	308	348	300	278	190	239	195	268	358
248	222	221	296	301	287	392	252	124	305	223
257	248	1	330	258	131	292	144	295	272	239
212	235	241	242	195	273	246	235	230	206	

224

1140.2_1185EK07	446	999	156	361	341	395	449	192	353	235
304	390	356	547	339	348	340	243	315	403	351
370	241	347	322	256	353	417	376	376	370	347
377	364	301	287	301	182	297	386	304	393	241
256	346	387	261	359	315	293	308	287	313	356
376	271	277	266	310	328	263	252	249	245	273
242	291	280	271	230	283	320	281	293	276	310
248	323	376	268	329	331	294	273	303	297	272
299	291	279	246	325	237	322	353	328	281	278
296	313	328	232	332	230	324	323	336	301	299
232	232	234	236	328	272	328	299	285	298	271
257	283	211	249	251	258	263	295	277	363	242
304	404	276	237	289	367	246	251	338	303	218
298	322	256	277	263	264	253	296	302	336	246
267	260	216	307	299	278	311	286	276	295	293
268	216	158	238	303	302	197	241	182	246	238
213	177	246	201	266	157	364	223	250	239	312
408	326	195	194	372	449	357	192	242	471	157
294	264	399	214	288	289	245	243	344	257	368
264	300	350	387	286	318	371	407	267	166	246
247	310	142	185	320	223	208	282	326	245	363
249	161	217	211	406	267	357	344	274	315	142
291	172	336	287	264	299	261	294	279	299	362
180	199	186	348	233	366	262	225	175	295	271
161	319	318	149	298	227	308	222	313	233	341
267	322	298	179	343	225	277	245	296	192	295
279	172	188	251	311	260	264	165	277	320	358
329	298	334	325	210	337	336	256	359	320	244
217	25	231	305	256	389	265	315	382	352	304
227	225	306	238	252	301	204	233	188	266	292
211	216	235	304	344	268	382	292	144	279	216
316	265	95	303	295	214	275	278	295	295	286
244	232	343	337	299	379	305	351	342	284	

225

1200.0_1135EC03	223	156	999	274	255	210	192	189	127	207
282	131	165	221	212	193	192	225	262	225	167
205	186	31	168	250	164	194	173	211	236	64
234	161	158	214	40	842	260	141	270	187	252
278	243	0	258	30	213	237	189	190	210	123
219	198	200	201	212	159	199	193	8	209	193
223	99	204	185	206	185	199	194	278	229	208
237	218	228	157	162	237	187	166	186	201	118
180	140	134	3	146	284	194	157	188	140	169
188	199	187	700	259	160	219	236	201	199	184
0	118	64	55	230	225	123	159	143	161	289
239	141	164	118	120	57	40	162	188	195	165
147	171	263	145	184	210	714	139	340	19	229
145	206	202	173	228	231	229	227	220	209	230
230	106	114	170	168	220	165	144	126	188	146
198	677	80	165	153	154	258	8	81	22	76
23	41	69	0	621	53	237	113	174	616	180
143	139	262	189	234	192	8	107	218	38	263
128	3	217	215	150	208	0	1	166	106	162
158	106	144	134	169	205	286	205	136	20	96
34	58	178	55	131	1	269	144	80	210	13
125	0	96	145	206	168	137	123	1	193	85
118	139	174	0	49	4	110	196	1	11	192
93	175	130	398	145	222	21	41	77	208	105
165	210	30	0	60	9	195	15	157	174	201
239	0	209	103	195	190	41	6	60	120	101
0	144	0	0	208	14	9	226	12	126	175
1	167	146	129	164	275	198	200	189	112	43
61	0	2	227	128	29	157	25	144	233	269
14	212	204	63	0	211	69	11	123	81	84
2	109	203	94	252	2	213	52	165	224	163
56	106	0	49	176	0	0	82	86	1	42
186	45	184	239	82	129	152	135	47	95	

226

1221.9_1185EK06	312	361	274	999	910	385	340	240	392	327
258	368	363	462	310	321	309	289	349	370	448
474	323	377	439	317	299	379	489	339	544	322
321	322	278	316	326	239	347	474	375	391	196
298	384	388	409	235	311	389	246	328	338	330
452	313	332	311	352	379	313	217	333	226	243
209	338	303	242	254	282	339	261	247	304	436
286	272	405	292	279	314	195	175	289	304	296
306	311	332	267	303	189	335	326	347	346	305
347	318	310	171	321	262	331	308	413	326	324
248	315	316	332	476	275	281	257	285	255	277
233	290	169	345	334	266	230	283	251	370	310
283	296	231	178	338	312	175	433	237	311	225
247	473	266	250	271	267	260	276	277	343	252
289	296	300	323	314	279	304	266	313	309	304
293	160	284	300	312	308	193	170	185	128	208
204	44	156	169	176	177	287	164	269	149	960
392	321	133	371	413	340	429	246	270	378	239
336	267	354	223	299	326	319	351	473	275	320
392	254	393	423	469	282	386	411	347	151	334
275	350	301	285	390	127	281	283	367	424	199
283	0	324	185	482	403	455	335	308	360	72
316	75	411	279	344	399	290	369	321	369	310
262	350	231	310	306	346	320	222	357	416	313
191	346	362	165	287	243	391	297	194	88	439
179	360	311	273	372	6	327	237	324	179	289
0	273	165	362	376	363	312	260	339	486	363
299	338	296	311	257	294	327	305	291	338	298
362	25	286	332	330	411	294	378	412	310	351
305	300	421	320	305	281	240	254	325	246	318
237	254	313	357	362	304	392	320	110	295	288
292	280	125	248	302	118	330	216	320	319	279
214	297	300	316	311	298	237	260	235	286	

227

1260.4_2011EC44	294	341	255	910	999	376	322	297	358	325
292	365	384	456	295	331	310	263	352	352	396
379	343	368	424	303	321	366	396	359	458	351
338	351	264	333	315	230	315	443	333	347	213
274	378	407	332	213	276	325	235	318	328	337
344	289	310	287	312	314	291	279	318	249	260
303	328	311	269	265	261	343	295	253	296	368
296	324	404	290	279	297	196	196	278	303	296
306	311	325	273	289	186	322	341	333	310	306
312	307	273	174	289	233	305	308	386	321	319
235	311	312	325	365	282	292	270	298	269	287
247	280	158	344	340	296	239	300	247	357	296
301	317	253	198	347	326	172	352	264	262	233
255	483	251	241	273	257	267	291	282	347	242
276	281	317	310	300	271	295	244	312	295	299
287	167	269	292	314	311	222	176	214	157	213
289	159	255	170	178	175	307	213	244	156	933
376	290	164	350	391	322	398	263	321	353	203
357	334	378	224	302	348	232	370	405	244	342
351	274	349	406	399	347	370	400	363	246	339
185	360	304	335	368	119	253	351	364	338	162
302	0	339	200	457	378	362	332	353	338	160
296	77	333	345	338	387	274	358	346	359	288
270	319	274	303	317	361	336	325	308	376	318
240	336	311	223	299	322	357	341	256	175	402
260	375	314	282	364	234	312	250	309	219	281
0	259	219	315	372	347	318	289	340	387	345
342	348	329	296	309	307	325	291	339	334	280
332	102	310	316	294	394	323	359	422	331	335
288	290	416	299	311	268	233	264	303	276	354
310	284	290	331	351	286	370	292	189	312	258
276	257	168	285	281	150	317	271	318	320	272
214	281	314	307	312	326	290	267	258	290	

228

1280.9_1164EK04	652	395	210	385	376	999	343	150	335	176
220	470	360	378	281	310	293	219	255	367	373
375	260	356	577	237	341	360	354	374	390	348
371	384	275	319	328	158	301	578	323	323	252
248	336	304	299	258	331	319	255	349	345	297
345	312	321	313	280	626	303	231	273	222	323
234	299	346	328	207	260	338	328	273	214	272
227	260	338	244	289	294	219	288	290	296	302
311	295	296	260	300	218	305	332	301	288	295
291	282	275	119	293	133	287	329	309	315	312
254	243	244	255	328	259	291	306	274	303	228
261	228	210	269	236	239	202	327	329	356	231
260	371	243	234	324	335	118	290	291	301	129
234	414	236	244	221	246	220	259	254	309	235
229	263	219	273	272	250	277	232	289	288	296
254	111	318	233	297	292	242	234	32	234	261
131	38	232	221	97	171	251	257	237	111	378
363	313	216	311	935	343	354	131	198	508	64
283	237	330	216	219	310	163	336	403	239	443
483	239	486	527	318	284	353	410	284	5	316
272	323	155	205	359	99	254	284	273	332	248
226	0	213	180	367	221	315	251	247	354	50
210	115	589	294	281	307	154	302	307	289	336
187	214	194	317	216	338	256	165	225	255	261
224	303	322	210	203	263	283	253	191	54	335
193	224	307	327	318	11	293	239	278	46	242
0	267	123	288	275	268	247	173	261	301	333
234	251	330	294	269	267	260	350	345	284	214
215	24	315	285	258	345	318	374	364	273	269
281	330	322	237	255	243	189	205	197	233	295
193	207	256	272	259	280	345	264	118	292	240
211	246	55	291	251	99	251	111	282	273	217
233	210	267	236	185	275	190	261	228	188	

229

1291.0_1185EK01	348	449	192	340	322	343	999	191	391	790
292	320	404	537	313	361	845	262	310	389	389
411	212	329	399	302	436	393	421	403	474	404
399	391	253	321	352	220	347	455	379	345	316
269	375	346	331	187	299	370	252	255	348	317
385	305	327	315	278	346	316	267	354	285	275
318	325	279	272	306	262	359	256	290	255	344
317	319	389	304	299	327	205	335	330	315	253
259	326	290	292	278	203	355	305	340	326	314
320	331	299	185	289	216	318	299	356	307	307
208	325	325	333	375	340	318	270	260	275	267
277	225	159	318	322	284	250	308	231	357	289
284	305	312	164	325	366	170	394	295	277	202
253	385	279	238	259	287	253	274	260	328	284
278	266	255	319	299	241	296	255	324	317	344
283	163	219	306	300	297	241	202	48	229	229
239	113	178	180	182	201	240	213	284	173	313
368	357	94	308	345	999	426	209	806	339	223
366	321	388	236	280	327	270	304	416	280	458
358	307	383	433	415	301	443	466	322	143	364
308	358	217	221	398	142	217	377	343	389	176
239	0	265	235	420	303	389	296	328	338	30
252	87	364	341	314	303	269	330	323	381	347
332	297	249	284	222	391	322	191	305	343	296
194	346	322	248	243	303	366	305	259	176	376
218	291	334	225	374	240	307	218	301	134	294
2	316	206	330	342	297	330	160	342	378	358
284	320	355	313	267	279	344	253	350	305	305
295	189	337	364	318	370	270	350	417	277	300
184	250	359	255	261	265	207	266	287	242	473
313	276	263	340	356	299	343	263	151	307	278
268	283	134	306	282	145	261	159	302	291	273
237	277	249	270	253	280	211	263	240	200	

230

1293.1_1164EK02	195	192	189	240	297	150	191	999	274	226
243	204	253	265	290	286	195	261	257	258	162
165	194	287	205	197	245	259	201	258	291	272
249	268	246	287	280	174	260	216	204	234	256
249	207	220	166	170	311	266	232	207	174	262
213	209	218	198	169	229	200	651	251	578	210
617	232	234	208	570	594	218	203	326	635	222
571	285	161	273	247	342	184	275	257	287	252
267	240	229	148	269	166	251	273	229	246	234
246	230	216	195	229	265	217	218	177	248	249
220	234	237	249	263	238	92	270	247	268	239
231	170	250	212	214	231	243	245	251	262	263
238	194	225	259	157	143	146	174	195	202	132
238	136	508	525	532	507	508	554	493	450	500
529	210	196	248	260	218	224	221	234	263	256
207	154	151	217	243	238	303	263	179	240	266
242	107	243	236	142	169	265	303	251	139	298
265	294	208	189	164	191	305	955	137	238	2
273	233	275	190	262	256	170	315	242	242	188
205	124	236	297	291	289	218	242	275	34	276
231	272	186	240	263	145	254	178	228	182	84
295	148	240	246	179	195	223	178	269	232	90
245	421	198	267	164	284	124	254	243	266	482
209	205	234	209	251	176	666	16	258	198	232
47	301	262	202	246	597	125	274	199	98	323
221	320	209	206	163	193	241	227	270	215	208
243	243	192	259	170	285	240	169	259	271	228
281	240	179	229	462	228	142	210	200	231	287
431	401	158	265	262	266	151	232	292	231	193
107	220	242	226	258	570	369	525	209	536	278
463	494	246	251	274	517	313	253	56	206	511
224	521	436	251	237	74	264	139	243	271	237
422	358	323	311	258	306	265	291	281	218	

231

1302.8_2011EC21	355	353	127	392	358	335	391	274	999	286
339	429	370	417	492	512	338	359	421	419	550
515	233	585	355	287	477	344	384	736	487	687
721	707	499	551	730	159	624	373	445	317	403
374	342	646	403	216	435	389	255	383	327	478
422	551	535	545	335	356	529	371	647	329	533
372	700	565	545	309	404	299	576	447	455	317
380	507	274	414	447	451	225	410	478	611	635
628	655	625	296	625	152	653	647	656	627	635
625	656	681	155	697	218	690	241	311	603	602
365	598	603	616	426	373	284	683	322	681	498
409	243	333	575	540	391	325	233	394	341	445
357	329	285	367	292	181	156	382	289	274	164
360	198	384	448	407	389	401	438	393	471	358
430	499	400	555	567	418	554	468	623	546	653
418	128	303	527	520	538	239	437	172	401	452
311	341	402	442	143	220	312	432	435	168	417
372	524	181	206	310	391	974	246	244	489	24
300	454	547	232	353	366	504	472	519	330	289
313	136	302	428	347	453	289	364	485	188	506
277	729	99	239	417	110	351	283	582	413	234
404	1	445	272	316	282	455	238	664	582	45
199	175	379	460	252	633	158	364	604	695	556
363	375	269	276	442	247	461	164	486	303	515
145	582	619	327	486	392	217	449	203	41	597
381	581	568	326	226	271	629	365	585	189	495
284	526	137	582	267	527	629	291	663	424	571
587	599	263	540	385	277	143	315	325	532	487
309	93	330	565	602	676	396	471	619	313	278
226	300	574	516	555	522	258	357	435	421	675
404	402	468	600	563	460	528	524	219	402	393
422	397	118	518	500	142	512	84	510	545	533
308	377	260	279	241	351	244	334	285	278	

232

1315.1_1164EK04	191	235	207	327	325	176	790	226	286	999
264	212	262	353	275	255	806	231	300	313	288
330	154	197	339	302	351	275	352	220	454	249
237	224	181	251	221	217	262	381	307	262	286
266	350	204	306	91	287	359	160	200	245	226
339	219	253	227	240	300	234	274	247	217	162
316	237	194	153	275	237	264	141	188	233	317
234	243	303	241	185	264	129	233	250	246	247
245	208	235	229	256	163	292	232	286	252	209
236	273	249	173	238	217	237	236	302	231	232
128	211	211	231	369	283	187	221	156	246	229
213	208	119	292	254	209	184	247	155	277	215
166	186	304	131	237	281	154	357	226	257	175
183	293	233	219	218	238	204	232	221	267	249
230	232	181	281	248	251	247	233	243	231	250
244	143	174	249	278	236	214	149	98	154	161
124	23	126	124	179	220	224	163	270	147	313
277	315	134	296	191	790	313	321	970	190	249
261	207	256	204	278	278	230	217	343	261	333
374	210	234	300	394	250	341	421	276	138	261
219	316	205	200	333	164	235	344	239	332	20
238	0	271	180	312	288	356	269	215	290	50
204	44	324	260	296	275	230	275	231	264	320
209	249	177	209	314	251	324	191	308	308	291
131	341	297	104	217	287	311	245	188	145	339
221	296	312	181	283	6	226	136	259	106	229
0	246	1	263	275	264	246	145	269	382	271
220	270	233	224	225	198	266	171	294	220	229
207	131	267	292	215	315	260	317	376	211	239
183	170	326	228	190	273	133	191	263	153	494
291	204	251	309	329	250	303	235	121	238	256
259	225	57	220	251	2	245	76	292	244	236
253	295	238	228	190	239	158	225	195	151	

233

1318.8_1185EK05	283	304	282	258	292	220	292	243	339	264
999	245	282	508	314	350	249	282	264	259	242
283	267	294	306	328	309	316	240	328	304	339
322	319	244	376	276	346	366	337	253	298	305
279	368	366	224	212	254	259	208	193	290	299
229	259	281	266	235	305	264	286	252	289	245
282	273	304	241	313	233	265	267	237	281	301
249	270	601	220	232	307	195	211	257	277	268
263	268	275	219	272	207	285	295	293	250	277
252	274	232	315	230	280	244	197	301	275	273
215	256	254	261	202	276	186	297	270	296	312
228	180	198	281	282	289	257	186	196	340	227
251	272	277	181	227	329	294	284	199	149	270
239	334	243	234	227	253	203	229	223	323	217
230	238	252	286	269	234	273	215	260	256	288
244	294	237	245	286	254	205	207	155	132	190
16	154	186	240	303	217	323	146	221	274	290
333	256	178	261	217	292	368	300	266	272	944
309	348	276	331	328	309	199	371	300	295	321
297	237	240	324	263	315	381	451	329	183	383
213	336	266	326	306	134	238	282	341	218	153
315	0	316	639	647	288	252	352	330	317	140
306	266	298	289	324	341	191	300	311	285	294
262	280	331	324	446	395	309	244	277	309	296
221	363	317	231	284	322	577	301	287	372	347
271	319	242	233	266	61	249	306	283	218	264
0	244	264	279	273	325	273	178	301	243	310
297	334	342	292	240	285	320	266	287	296	243
276	73	252	315	236	342	235	331	356	297	315
122	273	364	320	287	233	232	223	262	205	402
253	243	252	301	321	257	355	263	129	319	257
270	262	197	289	244	251	269	242	286	262	248
231	229	320	334	297	326	294	297	276	277	

234

1318.9_1164EK04	377	390	131	368	365	470	320	204	429	212
245	999	320	349	346	319	320	256	306	330	391
580	282	566	346	222	322	358	422	453	397	470
467	464	287	301	360	121	351	377	385	345	260
245	383	445	307	306	246	329	244	424	278	424
367	293	299	291	340	387	283	254	327	239	503
239	353	490	518	261	242	292	484	259	284	340
283	336	358	285	314	302	210	235	258	305	300
310	310	310	285	313	209	345	382	355	364	299
357	315	327	111	341	181	308	298	322	391	385
269	300	300	305	377	312	291	351	298	347	307
301	263	281	350	324	323	246	284	274	303	256
284	294	268	322	368	280	104	280	348	355	246
269	268	271	254	284	260	242	248	247	291	253
256	285	196	377	370	241	337	282	349	355	346
266	94	404	328	336	347	214	296	106	296	290
262	194	260	302	91	219	255	301	282	91	339
424	337	101	148	479	320	434	185	10	940	5
198	273	398	213	313	275	296	418	577	236	417
259	135	464	524	304	285	263	400	286	334	324
288	327	144	184	362	76	229	251	395	324	335
271	0	243	152	347	284	371	300	397	326	154
196	111	394	377	209	323	109	310	451	372	333
196	223	235	286	293	345	252	0	310	291	283
154	315	388	69	318	249	262	261	123	130	400
235	325	338	402	304	116	321	275	293	34	369
5	281	171	268	295	225	324	155	361	366	379
314	375	282	357	254	338	238	391	380	380	206
330	21	285	314	305	380	188	289	375	382	314
304	389	315	284	340	265	165	227	221	195	373
237	210	264	320	289	234	421	325	116	283	233
269	269	127	376	311	146	336	57	338	327	337
200	234	244	249	219	307	228	275	267	254	

235

1326.9_1185EK07	360	356	165	363	384	360	404	253	370	262
282	320	999	405	333	390	376	289	340	448	397
379	169	333	602	314	336	807	370	385	359	370
409	404	333	354	318	171	300	465	421	371	283
293	679	382	279	166	377	393	250	352	695	317
314	318	305	300	319	349	311	355	276	288	309
334	303	301	307	302	288	693	316	336	272	272
282	319	482	231	301	303	194	344	304	312	280
285	302	311	387	302	227	320	331	325	278	297
275	310	310	180	302	150	307	753	537	293	289
213	259	260	269	352	304	222	330	263	329	277
272	203	146	285	278	293	263	737	320	348	252
273	309	296	181	262	468	177	279	274	265	151
266	469	263	267	300	310	285	321	319	327	279
264	271	239	304	290	273	312	254	296	319	307
272	164	180	249	318	309	190	270	106	242	304
292	232	259	283	150	217	266	260	254	161	360
368	316	115	727	338	404	387	262	252	357	108
929	363	398	250	294	424	249	332	370	230	305
378	503	364	438	272	355	394	405	309	188	346
260	316	195	295	426	174	278	507	306	308	144
274	0	269	241	302	377	294	340	330	357	19
134	170	379	361	307	284	303	330	385	302	355
222	304	384	284	226	564	313	383	291	305	339
535	292	338	242	240	305	407	271	207	75	351
201	316	354	200	554	358	309	228	292	119	306
1	282	201	318	480	311	269	221	282	361	334
277	324	621	322	319	217	367	218	702	323	233
264	213	751	301	297	423	519	557	448	219	246
208	208	422	264	264	270	163	281	206	276	355
305	272	245	341	261	340	363	250	102	325	258
261	265	62	335	257	231	305	96	305	319	254
228	224	236	231	226	271	214	253	241	191	

236

1334.7_1344EC21	448	547	221	462	456	378	537	265	417	353
508	349	405	999	447	452	407	308	421	418	441
452	287	416	436	357	396	426	413	438	474	401
446	424	334	407	354	198	360	412	585	349	401
393	435	425	363	202	388	420	298	333	365	402
387	363	365	367	369	418	365	345	315	324	363
317	351	348	369	316	312	362	349	356	282	411
313	312	519	320	354	412	216	379	351	377	364
383	381	378	302	395	213	371	326	376	356	388
369	376	367	170	369	186	371	287	460	367	369
294	294	300	303	431	336	283	398	268	399	327
318	296	251	357	329	318	196	270	334	423	282
267	368	351	292	380	337	178	357	268	238	247
247	386	297	300	302	310	297	334	331	360	302
288	293	336	331	322	352	329	249	298	298	319
378	160	197	279	313	299	239	296	80	318	303
251	248	296	294	170	214	313	313	249	158	433
427	399	90	263	336	537	422	211	306	420	362
340	420	398	257	358	388	296	370	427	390	333
364	263	358	397	364	404	487	453	438	216	399
299	408	227	281	549	82	362	328	408	386	203
332	0	322	426	584	359	382	389	360	406	58
253	188	415	384	344	386	241	400	341	359	400
211	344	256	296	332	433	306	205	384	417	353
218	387	437	268	245	320	412	332	203	157	434
255	302	352	211	382	254	373	221	361	134	323
0	277	132	271	384	344	304	187	331	397	400
283	386	370	352	242	273	330	247	349	321	316
276	54	350	355	293	434	270	420	423	274	310
157	237	440	322	296	341	224	267	325	295	436
231	278	361	393	419	311	378	311	135	325	316
307	298	132	289	290	97	269	155	313	277	273
271	242	292	275	268	314	252	258	216	232	

1336.4_2011EC31	349	339	212	310	295	281	313	290	492	275
314	346	333	447	999	674	285	627	659	320	304
335	290	374	270	303	469	335	262	461	322	511
492	493	575	594	483	221	438	329	329	302	339
330	319	505	268	214	418	344	239	238	240	505
289	334	329	330	282	259	329	286	350	278	312
248	454	354	316	249	311	231	343	504	322	354
327	379	331	493	439	459	174	395	465	431	370
376	434	401	349	380	250	416	389	409	417	425
401	423	382	194	398	194	416	181	293	416	410
229	367	366	359	260	326	157	536	251	537	446
340	208	183	419	362	401	170	226	312	313	382
260	257	289	222	301	172	197	317	278	224	237
244	238	291	315	301	292	295	317	306	377	339
361	330	359	351	333	323	334	282	371	309	378
356	193	219	312	326	310	227	377	124	364	372
303	290	339	401	195	190	306	309	284	192	291
532	606	212	215	261	313	525	251	190	411	160
319	632	424	384	716	339	376	491	358	339	230
323	171	299	333	220	581	348	273	630	266	573
139	512	191	319	353	118	319	227	514	281	221
474	0	445	310	346	286	316	314	422	383	82
260	137	272	496	363	428	175	333	455	415	369
223	419	328	272	344	254	347	151	403	353	466
114	434	372	278	323	359	209	485	208	199	431
333	403	384	209	204	308	383	214	345	202	314
0	364	181	393	245	519	382	253	419	285	370
343	470	191	345	354	233	200	257	202	394	440
302	123	355	369	365	407	160	438	405	259	234
184	242	406	423	369	356	301	344	349	329	429
353	367	354	367	380	323	444	324	254	400	315
309	306	204	363	318	152	303	130	343	353	294
234	304	309	327	297	355	276	327	282	226	

1346.0_2011EC29	367	348	193	321	331	310	361	286	512	255
350	319	390	452	674	999	294	369	741	371	393
402	281	446	309	375	592	390	341	535	394	511
495	512	578	513	450	216	426	329	396	321	377
327	361	525	346	257	477	418	215	293	336	435
336	392	390	393	423	344	390	275	421	310	347
272	491	366	353	259	403	324	350	438	424	319
365	379	340	374	461	480	208	446	450	429	406
453	489	430	412	445	209	456	414	470	394	460
394	495	481	159	453	164	491	226	312	426	425
262	387	387	370	290	351	232	483	248	488	455
363	260	208	393	380	383	193	259	326	371	389
253	272	276	263	333	218	178	372	254	225	217
222	245	346	395	359	339	339	346	324	370	361
355	400	304	424	399	381	405	341	377	388	438
367	166	256	368	410	379	157	386	167	314	368
293	375	314	310	185	221	287	349	322	126	325
522	639	171	224	299	361	522	283	192	401	203
347	950	456	355	469	370	400	438	388	319	276
352	181	310	357	255	705	344	321	630	260	523
256	485	164	291	391	69	301	253	454	369	243
420	0	445	339	315	306	365	390	462	435	0
269	126	343	451	305	478	240	353	485	465	498
237	461	338	326	359	288	421	168	394	315	365
155	435	522	286	334	369	216	504	248	146	445
366	397	373	262	232	355	433	217	371	139	389
0	398	227	417	272	549	423	293	432	366	429
371	512	269	364	342	281	197	289	259	403	435
371	192	380	380	395	467	207	543	459	292	253
182	282	456	430	359	483	274	378	345	362	512
338	384	370	396	383	373	465	374	168	417	414
355	379	171	456	383	189	385	190	414	393	362
317	365	266	314	283	330	287	302	261	306	

1351.6_1344EC23	306	340	192	309	310	293	845	195	338	806
249	320	376	407	285	294	999	248	315	379	380
386	197	317	389	341	422	372	368	347	442	339
334	331	273	303	280	162	280	413	339	336	295
307	359	324	324	146	267	369	205	223	319	292
364	298	323	307	286	330	310	241	295	255	278
311	272	266	272	281	234	341	239	260	251	354
288	278	363	282	246	304	191	292	288	309	284
290	319	303	340	292	213	335	274	336	269	314
254	326	289	159	276	190	302	286	344	253	254
157	273	274	285	341	301	269	241	230	260	260
230	183	177	300	268	256	199	272	179	364	258
239	277	282	163	327	328	165	368	247	243	193
187	344	250	234	235	255	211	227	215	314	270
258	245	255	279	251	232	270	235	283	262	289
298	161	215	273	283	251	229	191	90	226	204
188	22	167	187	176	202	245	192	238	147	284
357	357	151	374	312	845	381	226	858	328	197
329	259	357	211	301	334	202	299	408	254	438
348	254	335	386	395	298	396	450	361	152	317
300	325	323	229	393	184	277	423	331	376	110
247	0	309	253	378	333	361	292	296	327	60
218	105	345	374	297	287	253	346	312	307	304
262	328	255	268	272	373	299	173	328	358	291
197	346	257	254	266	291	330	357	207	172	367
233	324	309	224	348	198	324	225	307	221	239
0	300	206	291	353	329	278	200	282	371	320
272	295	303	274	242	244	297	240	336	266	253
317	222	350	334	294	319	288	355	386	252	285
195	240	352	275	243	256	160	247	289	217	460
304	275	258	313	336	260	307	241	107	285	231
248	229	146	277	260	131	252	141	276	276	233
205	263	261	256	257	269	212	245	230	208	

1372.0_1288EC46	270	243	225	289	263	219	262	261	359	231
282	256	289	308	627	369	248	999	441	257	240
267	283	265	216	253	328	249	237	308	284	330
327	316	362	507	367	274	396	290	250	234	271
272	292	386	241	186	359	364	216	219	221	318
256	344	327	328	222	228	329	344	329	304	283
323	336	335	287	286	342	192	320	347	252	380
307	276	263	482	245	401	184	477	379	344	306
330	323	312	203	310	237	339	360	340	442	332
446	327	309	247	339	196	316	180	254	442	445
226	284	286	317	260	357	170	363	228	363	396
372	251	208	367	331	379	180	210	259	327	338
241	211	301	241	339	197	239	333	253	190	288
218	209	271	328	282	286	266	302	309	353	309
350	362	409	367	359	422	353	320	355	330	362
456	247	225	350	352	341	212	313	147	313	345
266	215	327	264	230	242	288	297	330	243	267
349	344	207	197	209	262	367	260	169	274	227
295	340	289	293	887	268	263	439	307	287	237
294	197	270	263	224	358	309	254	425	249	510
161	421	198	239	246	105	275	209	290	276	136
377	0	324	230	289	342	247	266	280	350	97
249	180	240	288	349	383	226	374	418	360	357
210	294	231	284	258	253	301	191	408	407	332
149	344	369	296	280	308	205	302	195	212	398
237	341	373	233	204	248	357	236	312	153	340
0	316	159	277	231	443	310	211	305	286	405
291	366	201	310	322	261	212	280	223	276	340
288	59	244	373	302	295	164	299	297	276	250
191	278	332	350	302	334	208	260	375	285	336
265	317	432	334	335	281	350	380	332	362	304
313	318	169	271	367	137	272	149	351	332	321
283	297	314	350	298	320	214	312	262	246	

1373.5_1164CC54	366	315	262	349	352	255	310	257	421	300
264	306	340	421	659	741	315	441	999	337	373
301	157	314	249	309	515	323	316	408	286	463
418	492	530	484	356	259	445	253	338	309	347
396	349	481	317	240	374	304	226	304	260	452
293	341	326	330	310	294	326	281	339	219	294
227	389	307	298	196	346	318	285	630	348	311
398	413	296	432	464	467	200	341	427	381	398
384	404	420	363	407	145	400	401	406	416	388
415	396	410	271	426	223	430	163	273	436	436
228	327	310	342	314	339	149	503	169	486	392
344	233	122	452	430	376	104	152	289	281	405
220	228	249	244	272	123	253	285	277	281	265
216	162	293	320	296	291	293	300	290	310	353
408	361	370	342	345	299	339	310	335	322	351
344	302	141	323	327	297	215	361	135	299	320
273	340	303	369	269	83	249	323	280	270	297
508	689	92	157	253	310	458	170	223	350	205
362	708	395	346	489	362	432	375	323	183	168
354	85	280	325	3	641	306	237	597	168	498
125	456	118	254	318	0	373	252	427	355	247
481	0	433	306	283	255	331	324	412	350	80
157	313	309	459	313	444	219	267	437	390	320
139	437	311	316	307	247	319	69	399	303	415
131	410	427	241	310	450	107	425	118	267	364
330	393	279	155	218	278	408	159	311	44	212
0	302	0	368	264	497	360	302	375	367	360
304	519	202	294	339	216	208	226	225	336	460
120	138	361	359	358	426	2	493	431	227	204
128	219	377	378	323	396	263	318	312	320	425
340	374	380	347	363	273	408	281	181	418	342
290	266	1	368	303	38	234	98	290	362	323
281	304	294	275	247	264	223	250	207	195	

1379.5_1185EK02	402	403	225	370	352	367	389	258	419	313
259	330	448	418	320	371	379	257	337	999	566
423	253	369	476	305	402	463	405	399	405	412
400	419	401	401	394	227	407	401	514	409	321
264	410	409	342	227	319	386	278	391	361	429
355	339	355	358	384	514	348	303	357	299	336
318	352	321	342	308	312	346	326	336	282	360
320	390	364	329	318	328	275	318	347	351	313
329	375	340	709	348	208	367	401	373	361	358
357	366	377	275	375	247	372	353	340	385	373
289	337	342	352	363	318	316	308	307	293	349
286	246	195	325	352	338	326	338	352	459	330
332	364	266	231	403	406	258	392	294	306	236
324	342	315	294	296	296	302	303	315	351	301
314	288	292	369	348	326	360	314	328	331	349
267	262	209	336	366	363	249	306	171	303	312
301	282	305	300	306	273	352	287	265	262	365
476	327	147	376	376	389	408	263	312	372	100
382	386	438	321	302	940	340	371	414	209	393
467	293	346	424	341	365	401	408	389	165	414
396	377	257	544	519	180	269	299	360	379	230
341	134	335	262	358	331	350	390	419	362	84
279	160	533	382	293	383	227	381	367	378	380
279	297	268	327	325	364	313	327	330	380	308
243	396	348	269	356	366	353	292	339	177	460
297	374	392	222	361	282	338	319	337	193	361
207	279	234	306	329	362	340	223	351	368	392
385	364	329	384	306	326	326	276	374	427	330
294	215	335	377	332	390	309	360	438	336	338
271	275	371	360	345	345	254	326	274	297	377
364	276	333	392	372	344	421	338	189	355	361
313	295	169	373	330	277	344	261	369	372	368
280	293	345	358	322	367	300	366	362	271	

1380.3_1164EK04	411	351	167	448	396	373	389	162	550	288
242	391	397	441	304	393	380	240	373	566	999
473	160	369	484	267	351	414	485	426	464	380
425	409	351	410	454	142	427	364	472	326	242
263	367	343	537	141	370	422	249	246	370	356
499	302	324	328	290	499	309	195	381	223	363
215	381	333	359	208	244	336	343	312	251	396
259	652	313	293	282	370	221	247	370	338	320
328	337	326	439	348	188	379	561	378	393	335
404	347	370	109	378	143	365	327	384	424	406
244	343	344	360	528	292	207	327	264	323	277
250	198	172	278	307	252	263	293	324	393	316
273	277	248	202	276	301	110	430	330	370	103
271	361	283	300	258	285	280	301	265	315	251
292	298	234	435	456	243	403	309	421	431	413
234	122	195	390	422	434	175	256	16	255	262
228	252	239	261	135	107	275	227	289	121	444
431	354	123	324	378	389	543	155	293	400	142
362	365	350	199	288	500	817	320	488	268	267
434	278	334	417	377	313	323	420	369	185	348
250	417	223	308	450	0	250	233	310	562	198
237	0	252	236	412	379	521	269	522	356	185
189	43	531	336	286	348	206	365	350	423	409
250	293	261	243	247	330	268	239	326	381	283
256	320	291	238	490	333	355	299	190	111	448
197	517	275	216	307	159	328	502	318	165	229
203	288	190	365	333	432	367	235	380	556	408
515	339	319	565	303	197	287	239	341	580	328
288	213	312	332	346	406	285	327	343	202	256
234	235	374	331	520	334	203	290	278	239	269
377	257	294	312	332	322	352	315	104	273	246
286	315	72	461	312	160	455	40	417	419	500
217	265	209	255	184	263	188	264	273	158	

1402.5_1164EK04	341	370	205	474	379	375	411	165	515	330
283	580	379	452	335	402	386	267	301	423	473
999	235	651	426	286	397	432	539	407	645	427
422	398	352	402	454	188	419	429	482	480	333
285	417	505	507	210	365	404	297	362	381	441
490	403	396	389	529	406	380	309	457	274	481
316	471	490	486	297	348	365	491	305	351	398
303	307	371	350	364	393	270	298	352	445	424
431	433	437	331	425	215	434	405	449	465	441
471	421	404	150	434	230	405	344	389	462	464
321	390	386	431	582	367	289	328	331	326	382
348	327	375	454	429	329	329	287	275	405	348
360	327	282	369	448	359	153	581	372	463	198
325	355	342	359	357	340	330	377	322	383	355
326	365	303	447	442	313	428	376	426	420	439
314	145	354	383	436	434	260	333	132	345	345
310	124	330	321	153	335	341	426	356	136	427
376	333	171	335	374	411	538	191	325	606	152
339	347	372	221	272	342	362	404	948	289	374
354	256	414	477	559	297	389	454	321	85	372
376	393	203	230	425	169	214	280	484	520	184
267	0	305	221	411	370	480	304	399	461	46
283	90	471	371	318	452	218	440	384	482	405
278	263	267	296	300	359	287	241	393	388	385
253	359	471	243	368	315	336	303	232	96	533
226	365	431	345	315	175	432	347	379	142	392
255	317	192	361	385	365	411	180	429	568	479
377	465	289	430	286	357	305	368	358	442	349
419	195	327	416	372	441	344	385	457	366	384
394	357	422	427	427	371	235	293	324	242	395
310	225	386	403	402	330	480	429	149	329	315
362	353	89	357	402	121	382	215	415	411	404
289	286	287	315	294	328	275	304	279	283	

1402.9_1344EC19	242	241	186	323	343	260	212	194	233	154
267	282	169	287	290	281	197	283	157	253	160
235	999	282	199	198	303	225	247	251	245	232
262	238	338	279	274	261	297	309	209	206	260
211	261	262	216	248	220	210	214	244	210	267
214	236	241	248	169	268	236	220	229	224	296
217	252	274	293	211	264	207	277	235	255	270
309	265	251	242	230	288	199	289	274	247	250
252	259	256	120	242	179	259	260	254	266	251
268	258	242	235	230	176	237	187	228	257	260
223	216	214	229	201	289	256	244	255	246	261
250	269	253	255	241	255	214	167	215	297	224
248	237	199	263	165	248	221	161	283	236	335
220	293	237	238	233	229	219	247	221	256	253
236	242	220	247	242	261	243	232	245	222	239
249	226	365	237	266	243	245	245	122	258	250
225	145	267	224	262	220	296	273	252	255	308
288	215	139	139	239	212	240	175	154	303	193
132	179	238	245	224	186	113	305	260	199	306
185	135	257	288	217	193	295	342	236	74	249
166	264	188	130	182	25	203	203	261	207	270
251	0	282	164	301	196	205	187	174	265	37
249	91	274	135	214	240	192	232	163	223	270
170	110	144	354	127	234	245	79	217	253	163
154	273	259	153	147	217	234	192	180	198	267
173	141	301	364	212	187	241	156	229	143	291
0	231	176	180	210	167	225	130	210	192	254
203	225	191	207	155	375	168	379	165	195	217
200	51	153	262	177	224	186	233	244	379	350
253	381	252	235	201	226	192	178	167	226	204
162	153	265	222	248	208	328	265	44	246	243
180	239	7	150	251	89	179	173	251	187	228
239	140	337	404	336	309	242	288	306	357	

1412.3_1344EC09	387	347	31	377	368	356	329	287	585	197
294	566	333	416	374	446	317	265	314	369	369
651	282	999	361	264	460	386	385	503	418	514
490	490	395	454	530	35	467	368	433	332	308
372	368	505	351	228	402	340	306	413	316	446
421	409	415	425	367	306	414	329	468	311	639
327	517	621	653	302	383	316	646	309	381	340
330	331	281	344	394	409	298	337	356	477	477
488	491	473	292	490	184	476	450	490	491	479
490	494	484	125	497	223	491	282	355	510	508
411	429	433	464	393	354	278	460	362	459	428
351	299	372	477	442	357	293	261	350	365	366
382	391	297	403	370	195	146	392	300	309	219
330	232	359	366	375	360	349	394	353	414	364
358	427	307	453	447	392	445	420	474	424	500
362	27	411	423	429	426	222	396	175	394	410
368	285	379	406	46	371	311	490	373	26	380
356	314	166	256	317	329	584	222	189	575	136
254	390	385	224	299	346	336	539	653	271	331
379	149	346	464	326	364	302	363	351	223	430
306	523	150	203	388	3	339	301	466	366	218
355	1	363	243	322	269	433	297	452	474	25
260	128	326	458	337	493	178	363	491	506	449
188	311	245	280	319	260	336	120	423	318	379
156	438	541	231	446	269	202	380	236	0	526
278	396	442	412	266	244	479	287	435	148	436
275	304	143	377	275	342	482	186	484	406	476
423	496	253	414	312	389	156	404	308	408	397
338	52	314	397	401	488	250	385	471	398	389
300	382	445	361	424	398	254	316	305	329	519
300	326	388	423	421	347	486	445	171	294	355
382	364	113	361	447	82	386	149	423	413	408
263	302	266	302	292	357	305	330	278	327	

1412.9_1164EK04	462	322	168	439	424	577	399	205	355	339
306	346	602	436	270	309	389	216	249	476	484
426	199	361	999	293	322	503	436	357	456	300
359	329	269	326	290	147	289	603	420	348	268
263	566	311	378	174	348	408	276	367	587	297
360	309	313	299	353	586	306	319	261	287	337
348	303	324	335	299	253	582	319	252	226	355
243	238	483	237	282	299	208	339	251	310	298
296	309	311	362	332	210	279	279	290	286	301
287	274	257	164	261	172	261	571	499	287	294
234	238	239	243	396	275	254	283	227	280	223
227	252	225	269	260	241	202	559	353	384	219
234	307	314	228	338	465	163	356	297	299	124
233	537	234	273	246	266	244	271	266	320	253
213	236	230	259	240	251	267	209	287	274	292
282	121	292	216	268	237	261	249	130	259	261
157	114	266	254	117	174	265	274	231	110	397
391	337	175	604	559	399	372	130	297	390	221
531	268	280	173	243	391	212	357	411	195	408
447	404	393	415	371	269	440	545	275	179	317
317	295	182	312	412	59	252	510	282	472	142
215	0	216	279	386	326	334	344	255	353	42
200	135	562	280	362	280	231	322	314	289	331
199	256	333	305	255	574	238	344	250	339	265
443	301	315	150	192	271	453	258	138	141	367
184	208	285	282	516	148	297	182	286	101	292
0	221	137	256	464	254	223	212	254	357	312
220	271	612	280	260	272	325	295	590	255	209
255	28	584	270	265	414	490	464	470	272	257
250	288	484	243	234	269	183	210	226	235	348
232	218	246	316	298	296	362	231	158	266	224
203	261	71	266	240	189	239	138	267	240	217
239	217	229	227	188	243	104	238	249	202	

1419.2_1135EC00	253	256	250	317	303	237	302	197	287	302
328	222	314	357	303	375	341	253	309	305	267
286	198	264	293	999	318	325	239	271	299	266
285	292	262	252	250	282	331	259	290	275	366
327	301	299	260	220	325	308	194	267	295	261
261	265	264	273	287	248	257	279	218	290	259
265	226	259	264	281	309	288	253	277	273	278
268	281	315	257	219	333	173	233	454	271	262
265	262	248	265	259	197	273	245	276	251	241
267	272	249	302	260	193	266	244	309	263	269
272	263	269	281	234	292	207	303	226	293	226
261	242	184	223	201	236	144	234	211	277	203
226	241	236	227	246	275	299	266	267	220	256
209	289	279	311	299	300	272	287	253	301	279
309	251	248	282	270	244	277	227	257	282	273
284	288	208	249	270	254	190	424	103	416	426
313	252	402	390	295	190	304	264	253	278	297
311	318	164	192	248	302	306	171	237	275	193
266	275	237	482	318	335	268	292	299	218	265
277	219	294	305	260	347	340	291	264	174	261
266	271	206	140	282	78	315	305	277	244	230
269	106	281	287	299	302	276	296	202	289	24
199	110	269	223	235	274	229	277	264	251	306
179	207	432	316	199	282	245	254	198	294	242
180	323	306	185	240	280	246	292	245	257	258
314	228	233	200	247	234	276	173	243	135	186
0	262	126	208	288	235	284	269	233	240	301
231	253	276	242	284	243	208	222	269	267	210
225	20	253	266	224	275	186	293	317	278	254
145	229	320	281	255	266	218	229	242	176	280
192	291	232	273	283	249	335	228	122	268	244
218	268	112	271	256	56	180	237	264	239	209
245	267	344	343	299	301	352	328	281	246	

1428.7_1344EC11	365	353	164	299	321	341	436	245	477	351
309	322	336	396	469	592	422	328	515	402	351
397	303	460	322	318	999	361	318	467	353	420
476	473	462	471	435	171	433	445	383	318	375
300	310	444	278	219	458	374	269	362	358	397
293	363	376	379	360	337	377	329	398	297	400
322	445	408	399	289	326	322	380	424	364	323
357	450	295	398	368	481	192	383	389	424	387
387	420	397	328	426	154	442	476	429	446	411
448	436	429	153	450	172	460	229	287	507	501
268	387	383	373	288	354	299	437	288	449	402
339	294	219	398	392	335	229	227	341	402	349
307	319	274	249	340	259	152	292	329	316	264
268	249	349	386	360	349	345	380	322	374	387
316	357	373	455	452	323	422	362	422	422	429
366	142	274	401	420	414	221	293	88	287	306
282	298	298	278	166	232	321	358	363	181	285
481	499	186	201	328	436	471	245	327	386	141
267	552	429	339	401	318	355	480	417	352	351
417	116	340	412	245	468	326	322	460	188	482
264	485	101	248	391	14	263	335	434	295	211
371	0	477	335	309	225	309	315	443	424	65
259	111	346	368	313	449	229	396	404	439	472
226	398	304	361	264	287	373	98	347	313	378
150	445	414	367	388	384	219	418	197	49	473
314	443	425	286	250	308	390	307	345	49	383
21	392	164	387	262	493	395	220	418	311	436
429	446	320	428	308	303	210	299	317	425	415
369	137	300	428	371	450	169	424	469	322	314
225	302	439	360	432	383	241	322	375	335	498
400	322	366	396	394	362	466	398	209	406	337
350	342	180	401	383	110	392	209	437	389	435
281	329	315	324	265	345	290	351	289	257	

1440.4_1185EK03	386	417	194	379	366	360	393	259	344	275
316	358	807	426	335	390	372	249	323	463	414
432	225	386	503	325	361	999	403	404	380	377
416	435	375	378	328	201	324	425	486	416	298
310	608	453	309	185	348	391	288	364	594	359
370	350	355	357	375	365	366	343	294	282	347
349	316	356	344	301	306	597	348	302	309	315
298	345	513	263	314	355	191	354	299	333	310
320	321	340	411	345	242	330	377	348	325	321
334	350	353	200	343	172	345	592	464	350	347
301	272	271	284	387	298	297	322	274	314	314
307	235	203	306	324	309	267	561	342	381	262
303	372	272	249	329	417	196	325	314	265	172
294	444	258	305	327	313	287	333	315	357	337
253	287	264	342	332	331	363	262	307	368	318
315	185	191	284	363	350	206	299	134	239	309
290	252	269	285	180	217	298	297	275	179	354
423	311	139	610	347	393	365	239	204	407	172
781	334	390	300	261	399	299	361	408	295	344
405	440	426	469	294	370	389	406	379	193	383
316	370	193	243	489	160	315	461	341	330	206
275	0	293	295	366	376	386	407	316	365	105
174	210	394	370	331	327	228	342	350	336	373
242	278	405	312	335	528	330	302	279	321	329
459	337	368	239	275	329	400	304	232	85	379
264	316	385	214	484	302	345	284	317	120	309
3	322	199	323	436	290	300	254	301	346	376
283	358	541	329	275	231	364	210	599	322	290
254	36	585	345	287	473	486	513	455	232	277
194	192	426	352	311	292	228	281	288	280	361
331	271	293	362	307	338	376	265	122	293	279
249	302	84	334	276	182	346	155	364	368	284
239	258	250	247	196	272	213	259	243	216	

1441.4_1344EC30	326	376	173	489	396	354	421	201	384	352
240	422	370	413	262	341	368	237	316	405	485
539	247	385	436	239	318	403	999	347	638	307
334	343	267	295	358	147	337	395	476	372	228
258	388	376	569	234	326	356	268	298	401	306
635	313	329	312	428	369	309	244	354	241	323
238	344	333	323	246	282	388	319	251	302	319
281	232	376	230	321	296	220	259	278	311	323
334	318	324	346	349	282	306	315	326	358	291
364	290	285	118	300	202	291	353	400	341	344
235	308	307	331	709	300	232	235	302	232	262
257	251	201	295	304	250	282	350	314	370	264
318	308	305	250	368	329	120	575	285	370	233
314	331	264	258	293	287	258	290	277	342	253
253	290	220	297	298	301	301	239	310	322	319
303	122	186	267	319	317	235	227	99	236	234
320	223	222	228	128	242	306	262	273	132	470
422	345	143	376	361	421	401	220	263	477	96
382	289	311	230	248	336	419	302	569	204	304
336	319	355	394	569	309	371	451	268	275	309
283	322	257	216	409	118	226	288	333	624	220
210	0	237	222	439	312	636	339	276	345	214
232	91	449	289	292	377	190	378	272	360	324
152	234	216	287	247	356	277	225	374	322	272
265	300	356	234	244	292	349	251	254	96	405
184	231	327	209	356	226	330	217	327	114	288
1	232	240	270	380	278	319	254	341	690	377
225	322	341	320	272	246	254	238	326	314	293
339	26	308	334	304	354	285	361	365	271	267
281	228	324	306	244	285	185	243	291	199	257
246	214	315	340	276	309	340	289	139	273	252
238	281	62	262	264	183	284	213	318	302	245
198	267	253	250	225	278	274	265	244	245	

1453.0_1344EC12	417	376	211	339	359	374	403	258	736	220
328	453	385	438	461	535	347	308	408	399	426
407	251	503	357	271	467	404	347	999	353	967
962	955	425	511	596	257	541	387	427	350	312
305	340	635	312	240	368	345	264	367	325	444
359	490	495	502	309	299	491	309	502	317	561
308	589	593	567	300	344	307	595	432	368	287
361	455	339	352	472	394	209	355	410	497	507
518	538	510	316	539	167	640	503	638	497	525
501	646	660	167	649	138	662	275	314	502	495
347	514	512	491	308	413	309	635	269	634	410
414	265	249	518	480	360	314	290	367	377	342
320	360	306	294	316	318	158	275	280	278	168
343	284	366	414	379	356	370	391	366	396	354
360	404	399	525	516	353	521	374	540	499	569
371	167	303	441	495	493	230	334	104	352	356
301	274	320	347	171	189	326	321	366	176	345
447	479	176	251	339	403	725	228	187	482	169
325	472	543	276	358	360	361	458	415	237	351
351	227	404	502	280	472	349	349	416	248	506
325	621	166	225	389	114	273	260	577	285	253
325	0	321	291	367	273	382	356	622	536	26
271	120	336	468	336	508	223	299	563	571	462
353	345	311	326	393	298	373	242	342	313	465
217	506	549	266	360	312	241	406	247	68	496
361	466	556	317	287	333	523	311	496	91	489
7	537	138	555	287	449	550	251	587	305	516
444	533	276	478	317	305	290	336	285	491	350
350	183	353	504	552	596	342	448	554	319	335
176	324	533	462	459	454	266	343	308	364	584
348	315	337	471	454	411	484	367	176	388	365
307	359	83	519	370	124	463	152	481	501	413
260	354	296	337	259	358	281	373	321	274	

253

1456.9_1164EK04	388	370	236	544	458	390	474	291	487	454
304	397	359	474	322	394	442	284	286	405	464
645	245	418	456	299	353	380	638	353	999	367
355	339	305	349	437	224	415	444	493	531	282
286	386	430	521	242	358	468	273	334	380	358
561	441	441	444	557	360	435	313	447	290	331
327	435	340	336	303	340	361	360	289	358	419
267	319	395	257	306	321	240	307	271	402	420
432	410	452	350	454	250	376	427	382	429	393
430	362	359	203	390	227	364	323	459	429	429
308	357	361	410	658	317	310	275	317	269	334
316	358	280	385	389	292	321	327	356	335	317
360	334	310	310	554	349	199	685	368	431	214
336	341	303	347	313	289	322	352	334	349	279
303	340	292	371	376	351	364	331	399	358	393
364	185	230	332	378	381	268	285	82	291	298
290	204	280	295	169	226	348	350	319	159	504
357	269	172	329	387	474	524	279	344	431	145
323	294	348	225	270	347	436	315	639	207	357
309	280	354	416	925	317	434	474	282	262	321
497	385	239	289	432	301	273	331	397	540	244
261	0	296	238	451	437	598	339	343	491	194
363	98	460	341	345	469	239	453	364	448	401
252	250	291	289	281	382	334	258	389	391	414
271	375	452	247	331	271	350	293	221	151	553
207	336	406	242	375	269	430	277	412	190	380
4	275	236	355	437	330	386	294	413	662	471
345	392	350	439	285	285	290	249	358	418	308
352	185	304	391	346	434	382	360	478	310	338
352	242	498	368	369	368	183	288	358	326	378
294	253	386	440	406	308	429	396	156	326	260
329	301	90	313	352	188	379	201	387	400	361
253	293	286	293	243	320	256	301	267	298	

254

1461.7_1135EC00	386	347	64	322	351	348	404	272	687	249
339	470	370	401	511	511	339	330	463	412	380
427	232	514	300	266	420	377	307	967	367	999
931	923	433	489	538	59	471	360	439	319	318
312	329	624	301	215	397	378	227	393	296	455
344	455	457	465	347	297	458	314	484	311	531
288	545	589	541	277	329	306	574	463	337	287
360	429	308	362	438	366	193	365	401	492	482
495	527	479	358	515	137	627	471	628	460	517
468	632	663	62	650	118	664	243	284	478	472
319	510	511	483	321	391	289	610	285	609	433
400	262	255	528	473	353	220	248	364	319	347
290	320	283	301	307	202	62	268	293	300	150
280	224	356	403	366	341	369	385	361	385	350
386	411	377	489	492	357	485	363	502	464	532
346	49	251	414	449	460	227	354	125	353	377
338	241	319	377	49	190	254	331	337	57	361
397	461	92	221	318	404	678	260	205	494	23
281	442	556	266	359	352	316	423	419	226	321
337	96	356	485	288	523	317	325	463	240	515
316	574	224	226	408	1	288	263	602	261	248
423	0	350	289	336	270	344	330	586	492	0
226	148	348	453	334	496	168	299	578	543	423
300	389	275	281	389	266	339	68	368	291	488
188	503	559	340	365	296	180	379	139	3	454
343	456	567	263	275	327	505	259	474	20	477
1	534	129	526	241	414	546	264	571	298	497
417	526	249	480	296	235	142	243	277	492	349
338	185	328	474	530	597	351	445	588	269	284
197	234	508	452	437	444	276	340	329	353	628
320	364	334	501	473	413	439	371	192	378	360
311	350	62	484	359	43	415	109	438	472	398
238	338	232	266	207	321	167	307	204	236	

1464.3_1344EC12	417	377	234	321	338	371	399	249	721	237
322	467	409	446	492	495	334	327	418	400	425
422	262	490	359	285	476	416	334	962	355	931
999	979	433	498	577	261	525	383	422	347	316
303	354	641	305	241	378	332	259	355	334	450
349	485	489	496	320	297	487	305	487	313	576
304	575	608	584	314	347	314	605	420	345	300
329	455	349	360	462	405	215	350	405	505	495
506	524	496	341	541	168	654	516	652	487	514
489	660	668	196	656	142	666	279	315	496	487
348	501	498	479	320	423	320	652	261	653	420
425	286	232	496	469	364	301	304	361	389	353
306	381	294	282	322	302	186	302	290	282	172
331	292	372	386	376	360	361	376	345	392	339
360	386	392	534	517	350	521	341	533	509	560
370	178	279	436	518	510	224	328	104	349	350
309	266	316	339	182	189	314	313	363	174	336
438	482	159	260	333	399	725	232	199	482	181
342	425	531	278	351	374	340	452	439	242	357
374	260	404	521	257	488	348	329	427	193	500
303	617	161	236	377	97	260	290	560	284	244
359	0	343	308	361	281	369	360	617	528	25
260	122	342	471	311	508	226	293	567	551	462
404	348	313	312	413	312	366	214	340	317	478
230	513	539	298	368	315	257	395	242	101	516
368	463	545	292	286	342	502	297	485	80	476
7	566	148	565	294	402	534	237	559	323	495
443	547	285	477	330	299	297	317	310	497	348
346	184	360	498	538	595	329	439	536	314	328
199	303	532	464	454	447	254	349	300	361	603
371	328	329	470	470	389	482	364	180	392	351
317	358	94	559	371	127	469	203	503	524	412
279	334	290	317	250	371	261	357	300	259	

1467.9_1135EC00	410	364	161	322	351	384	391	268	707	224
319	464	404	424	493	512	331	316	492	419	409
398	238	490	329	292	473	435	343	955	339	923
979	999	429	491	557	193	497	379	415	327	312
303	355	645	305	248	362	331	242	376	314	450
343	470	466	471	312	312	467	305	485	322	565
311	563	596	574	315	337	334	594	461	342	288
351	459	317	376	472	398	185	361	395	492	484
498	515	485	338	535	155	662	531	663	466	502
472	668	682	134	665	127	681	262	300	487	480
327	505	503	481	318	407	295	648	265	650	428
408	267	230	494	470	354	269	271	364	365	352
289	354	294	277	303	262	132	287	289	285	157
304	259	379	387	384	364	371	384	350	387	337
358	379	380	519	503	345	498	332	506	481	535
361	137	269	412	498	488	219	320	106	337	338
321	252	309	329	144	187	283	320	333	156	335
429	473	172	236	352	391	699	238	177	492	89
333	447	508	272	356	384	317	438	414	245	321
379	202	396	527	254	549	328	324	416	204	488
279	607	155	218	377	105	255	308	555	284	254
423	0	352	287	337	262	346	335	619	517	21
209	126	359	466	272	522	191	287	600	548	469
371	347	328	321	397	279	365	97	334	292	467
208	498	543	306	377	311	176	384	203	95	465
377	459	560	295	245	336	491	314	472	96	462
7	565	137	561	264	395	539	236	546	306	496
429	553	253	493	329	269	232	298	276	516	351
352	189	368	495	546	616	329	432	553	291	289
199	290	526	456	459	447	244	370	304	375	596
357	331	318	464	451	399	456	345	176	375	340
291	341	86	537	351	80	451	192	479	499	401
257	318	265	302	201	330	259	321	222	272	

1475.1_1288EC45	329	301	158	278	264	275	253	246	499	181
244	287	333	334	575	578	273	362	530	401	351
352	338	395	269	262	462	375	267	425	305	433
433	429	999	498	499	200	434	281	335	277	331
324	299	441	292	195	424	398	206	264	236	430
282	368	383	386	311	339	380	285	431	252	360
268	444	384	370	242	345	230	366	413	341	327
319	339	275	466	339	458	195	339	369	443	396
389	381	405	324	410	167	410	432	405	488	391
489	407	387	245	403	152	398	198	278	507	516
310	384	391	406	298	326	291	427	270	424	376
310	239	175	415	384	327	219	222	314	428	404
305	263	263	238	278	149	232	271	286	276	244
257	166	359	370	392	349	351	404	343	422	330
327	330	325	421	408	319	415	333	408	409	435
338	223	267	391	397	374	222	314	172	303	305
262	243	292	267	239	153	308	271	365	245	259
415	436	187	192	271	253	482	202	163	316	114
307	539	447	300	496	339	351	485	371	359	264
303	178	258	351	204	443	293	238	947	230	521
219	556	203	310	358	0	315	222	417	311	185
476	0	502	226	305	340	290	279	418	390	24
217	115	334	503	263	455	132	365	422	459	434
279	405	312	277	421	205	330	82	394	310	474
130	446	374	399	353	301	188	442	186	204	491
281	409	485	268	198	311	416	342	367	213	413
246	408	130	374	251	455	389	235	406	308	456
361	435	205	377	289	254	194	281	264	391	416
339	164	325	421	394	431	229	350	382	272	268
266	267	400	404	370	373	273	322	344	340	429
314	285	445	332	308	354	436	401	241	425	328
362	333	189	347	404	168	361	212	404	364	357
269	324	278	320	304	332	233	350	266	278	

258

1488.5_1288EC44	358	287	214	316	333	319	321	287	551	251
376	301	354	407	594	513	303	507	484	401	410
402	279	454	326	252	471	378	295	511	349	489
498	491	498	999	568	236	487	356	463	298	395
311	297	497	317	164	437	420	293	304	270	544
340	510	528	531	361	320	531	305	483	306	381
284	520	425	388	296	373	252	403	450	350	289
391	424	311	433	437	470	232	364	466	466	478
512	464	502	364	490	225	477	486	475	545	457
546	475	441	156	450	185	446	210	273	550	549
378	483	489	501	337	386	252	515	338	518	442
430	237	237	495	449	459	240	238	402	385	487
387	289	276	288	300	152	156	354	296	230	189
271	180	329	391	341	331	338	362	345	467	349
425	390	407	434	422	387	425	424	485	410	486
418	157	239	427	403	400	170	405	321	474	418
420	396	455	440	194	234	313	462	374	139	325
517	529	123	225	299	321	556	284	228	355	172
346	493	504	299	582	419	318	570	438	358	255
390	179	309	365	226	545	273	248	536	291	967
202	607	108	254	433	107	329	209	441	333	185
494	0	402	314	291	286	335	253	460	552	46
210	100	345	475	324	549	156	339	540	521	471
216	404	381	239	343	227	350	151	463	355	491
155	428	486	435	440	395	221	469	254	86	533
328	491	441	266	201	345	551	345	505	210	334
285	456	104	493	221	536	473	264	503	303	484
440	535	207	433	355	222	163	276	254	446	525
351	203	313	494	457	435	233	501	478	248	223
262	267	456	472	387	418	271	320	403	320	476
330	410	407	395	371	387	414	461	330	408	389
423	363	165	380	475	200	350	147	414	399	407
285	339	240	288	260	319	216	339	279	240	

259

1494.1_1135EC00	344	301	40	326	315	328	352	280	730	221
276	360	318	354	483	450	280	367	356	394	454
454	274	530	290	250	435	328	358	596	437	538
577	557	499	568	999	44	821	403	400	306	332
336	326	648	368	183	397	332	267	318	299	552
357	742	748	751	295	386	744	355	827	297	516
348	878	534	524	288	385	275	544	363	408	284
446	544	253	444	411	485	248	384	519	738	832
825	759	822	311	805	154	678	714	707	838	751
838	681	711	82	725	162	713	258	274	787	787
361	705	713	788	377	486	256	556	376	563	518
492	232	336	634	614	470	292	243	385	388	628
372	352	295	368	298	166	76	364	281	248	139
309	172	458	545	469	442	464	495	438	508	449
502	624	458	679	695	462	669	596	780	647	781
492	35	291	674	635	650	224	443	211	456	454
399	419	448	485	78	291	342	493	549	47	355
410	427	163	175	304	352	738	243	141	383	100
288	432	561	249	359	344	431	448	443	281	277
301	167	262	373	343	438	264	288	389	225	566
250	904	84	247	341	139	310	298	587	373	245
415	0	454	247	334	258	371	256	745	808	36
206	178	434	470	285	748	195	432	661	847	613
328	408	304	236	478	224	404	86	636	276	655
144	628	671	493	633	353	222	426	182	46	667
307	752	594	305	212	333	822	464	784	118	596
443	555	111	610	244	482	761	242	772	367	723
714	678	206	613	342	255	180	298	263	586	640
448	239	344	588	641	747	451	529	733	289	254
185	278	708	562	671	619	286	444	629	473	621
470	402	599	639	632	518	456	661	307	543	472
585	488	204	522	629	139	602	101	650	648	658
310	502	272	283	265	322	254	347	265	266	

1500.0_1135EC03	205	182	842	239	230	158	220	174	159	217
346	121	171	198	221	216	162	274	259	227	142
188	261	35	147	282	171	201	147	257	224	59
261	193	200	236	44	999	371	134	262	177	311
304	225	0	212	172	254	231	202	244	215	142
199	261	261	250	200	106	275	214	6	209	245
225	120	244	237	195	246	258	242	301	252	195
257	283	221	210	200	289	220	216	247	248	181
216	157	173	2	180	318	254	193	245	178	166
229	265	227	801	313	232	267	285	172	245	226
0	165	78	103	263	281	107	219	169	225	323
290	136	218	176	165	3	113	166	172	227	231
170	189	297	212	199	218	814	127	371	1	253
193	200	267	216	291	290	274	290	237	269	282
290	164	256	205	197	251	205	205	196	237	229
244	764	153	223	187	194	295	53	0	0	141
4	0	128	0	674	65	275	0	213	712	191
127	177	280	148	174	220	6	93	202	44	320
132	0	214	252	238	206	0	0	144	0	168
151	126	148	166	144	228	249	129	171	6	77
20	0	183	42	118	1	271	99	56	175	237
178	0	90	201	202	171	163	84	0	236	65
172	169	146	0	44	2	130	230	0	8	212
127	24	118	397	0	226	23	43	141	202	0
204	203	2	0	86	0	185	79	197	175	234
223	0	245	156	209	135	38	6	62	91	96
0	226	0	0	174	7	6	230	9	113	236
0	192	166	120	181	311	223	257	242	116	7
58	0	1	283	218	2	122	5	233	286	277
0	257	230	168	0	249	67	6	120	176	0
60	151	245	101	311	1	266	13	0	266	201
0	150	0	73	221	0	0	177	77	0	4
210	3	193	287	123	167	214	173	151	145	

1502.4_1288EC34	361	297	260	347	315	301	347	260	624	262
366	351	300	360	438	426	280	396	445	407	427
419	297	467	289	331	433	324	337	541	415	471
525	497	434	487	821	371	999	367	393	295	380
400	341	586	333	195	441	372	245	341	323	519
335	672	682	676	309	379	678	378	713	303	488
349	750	485	492	288	398	315	487	405	387	344
391	504	333	412	381	496	240	382	497	629	730
727	655	719	292	712	201	617	643	640	740	632
743	622	637	351	673	196	646	313	337	715	711
334	619	622	690	349	458	244	550	354	547	567
487	245	328	590	574	444	280	211	379	421	586
346	319	364	357	346	223	313	294	354	266	219
309	256	431	513	458	439	440	500	442	477	440
489	553	410	600	607	474	575	518	673	573	685
471	302	266	589	537	545	269	397	189	410	420
387	394	409	418	333	300	357	474	504	318	332
390	409	241	180	283	347	651	197	171	340	212
254	379	574	277	345	335	409	392	416	258	287
293	127	272	384	320	439	359	325	315	219	481
252	799	87	241	312	44	344	253	556	325	256
425	0	427	298	399	299	333	327	639	715	195
240	235	428	383	270	689	207	444	576	749	580
325	353	264	359	456	272	354	119	608	323	616
127	611	635	411	591	266	271	366	198	123	630
364	666	541	278	270	267	743	444	700	140	532
429	496	141	561	285	401	677	240	679	335	673
646	671	262	565	281	318	199	308	266	538	603
430	117	288	605	587	663	389	516	641	332	297
203	305	655	528	613	597	283	400	586	428	560
439	356	620	606	644	472	472	601	265	559	471
523	483	190	468	552	137	528	154	574	571	595
367	461	298	340	280	333	238	335	248	284	

1510.5_1164EK04	511	386	141	474	443	578	455	216	373	381
337	377	465	412	329	329	413	290	253	401	364
429	309	368	603	259	445	425	395	387	444	360
383	379	281	356	403	134	367	999	367	323	288
309	415	333	345	221	386	372	271	419	445	327
343	382	393	388	316	500	385	301	356	273	367
297	365	385	367	278	303	425	371	284	265	402
276	287	441	288	267	353	226	367	290	416	360
387	421	373	303	407	210	356	386	354	384	421
388	342	333	140	334	145	337	395	407	398	397
235	282	284	308	373	309	334	320	246	315	294
295	293	215	334	312	259	244	366	335	450	317
264	338	329	233	341	451	130	308	294	309	234
264	549	286	348	283	294	278	320	298	360	310
273	315	334	367	367	314	352	290	341	368	358
323	96	307	321	355	348	222	251	86	230	256
172	61	219	240	89	212	288	265	306	102	455
422	352	208	376	544	455	399	210	318	384	197
387	282	314	208	279	324	240	375	431	276	480
436	325	414	441	374	269	374	506	272	61	345
292	409	248	283	343	153	284	512	339	362	210
308	0	320	350	437	330	323	310	358	407	27
296	110	550	319	355	383	263	380	330	396	427
256	275	209	422	241	480	306	275	347	387	357
291	401	372	256	261	275	389	263	225	140	477
166	301	363	292	444	14	394	245	393	154	353
2	305	109	297	398	279	311	126	334	342	441
314	342	470	367	266	286	275	330	424	322	285
305	36	380	322	311	454	429	365	511	310	314
234	322	534	299	334	320	184	239	340	256	442
256	220	376	420	419	351	404	367	203	343	289
316	304	163	325	324	172	337	66	358	330	302
257	273	309	300	265	330	196	328	326	233	

263

1519.2_1185EK09	353	304	270	375	333	323	379	204	445	307
253	385	421	585	329	396	339	250	338	514	472
482	209	433	420	290	383	486	476	427	493	439
422	415	335	463	400	262	393	367	999	407	240
213	368	421	429	204	326	320	308	280	302	368
437	334	348	360	377	464	345	259	358	218	390
231	352	408	387	240	256	337	391	295	283	307
288	378	349	237	312	342	187	259	276	333	265
275	306	310	466	300	187	377	403	362	357	303
358	351	316	199	326	176	335	317	343	387	362
232	320	334	361	498	325	340	290	289	290	301
267	262	176	306	327	244	251	331	261	413	271
289	381	300	214	371	352	194	464	351	353	152
276	342	273	250	275	284	259	269	259	319	267
246	255	245	373	364	232	352	285	339	341	345
263	206	229	339	349	353	179	241	36	239	252
154	58	190	248	196	204	283	221	279	200	385
396	369	68	388	331	379	481	225	286	407	199
376	389	382	261	306	473	388	442	479	314	348
373	281	372	454	429	337	395	425	401	117	464
291	374	289	347	986	124	176	239	337	457	147
284	0	280	269	430	301	485	324	409	373	150
245	57	506	437	375	367	206	392	381	390	376
269	307	280	261	371	360	335	238	369	303	339
226	399	301	266	316	341	324	341	231	171	491
278	379	341	245	298	235	314	327	311	122	290
12	323	214	345	325	351	359	138	350	538	367
348	354	348	391	307	299	333	281	395	372	275
313	179	356	363	327	383	332	356	403	264	316
299	276	372	290	337	261	221	254	280	214	385
318	270	328	313	316	311	400	332	152	350	227
287	249	120	338	315	210	343	211	378	364	328
214	255	229	273	244	311	238	276	251	229	

264

1523.1_1164EK04	347	393	187	391	347	323	345	234	317	262
298	345	371	349	302	321	336	234	309	409	326
480	206	332	348	275	318	416	372	350	531	319
347	327	277	298	306	177	295	323	407	999	270
276	362	381	306	244	343	397	261	305	374	314
395	266	268	263	516	326	252	282	297	232	304
270	286	313	303	277	252	376	308	277	248	352
265	298	393	254	322	324	260	276	249	293	255
259	275	266	353	299	255	324	303	315	285	271
290	305	290	235	290	220	303	329	412	302	302
279	255	258	276	366	305	303	245	332	236	266
275	347	288	273	293	290	302	338	248	346	246
319	351	290	307	607	346	230	553	363	392	179
319	348	276	272	305	327	280	313	319	329	286
282	260	298	303	301	285	306	246	296	312	298
277	195	208	230	293	303	249	231	98	231	237
184	129	215	248	184	219	312	277	215	155	371
362	318	149	319	323	345	350	234	242	369	157
368	272	289	221	255	337	277	278	489	190	287
370	219	382	443	486	291	425	366	274	276	274
560	283	253	283	383	781	254	250	333	316	238
224	228	242	207	343	375	401	321	268	307	8
301	73	356	264	317	285	211	392	259	314	314
203	260	244	248	205	347	272	180	253	333	275
234	260	321	211	239	273	323	288	205	163	350
202	279	297	206	383	197	260	280	246	171	305
2	261	245	304	422	287	293	186	290	382	341
293	301	366	331	232	282	290	238	358	333	221
312	154	352	284	267	329	295	313	344	272	277
325	228	349	272	280	263	262	274	225	253	276
278	256	263	333	307	307	346	274	159	248	241
235	260	122	294	242	216	298	198	299	326	284
248	224	307	271	259	295	283	288	281	243	

265

1526.0_1185EK10	267	241	252	196	213	252	316	256	403	286
305	260	283	401	339	377	295	271	347	321	242
333	260	308	268	366	375	298	228	312	282	318
316	312	331	395	332	311	380	288	240	270	999
408	331	335	197	195	327	432	204	196	268	332
210	318	321	318	226	367	310	266	346	254	272
282	304	316	272	280	292	272	282	341	384	351
309	267	322	302	271	368	179	222	293	306	264
278	291	300	290	291	227	342	344	342	384	287
380	324	311	305	299	269	316	197	418	386	389
182	310	313	333	181	250	168	289	278	283	321
258	236	200	353	353	321	205	147	137	358	319
255	254	241	218	218	269	279	261	190	150	248
236	296	275	285	264	283	261	293	265	352	265
311	313	388	318	314	339	300	267	296	295	303
368	264	244	312	308	293	203	278	160	153	266
119	29	192	257	249	196	330	245	294	254	226
329	304	137	262	237	316	403	306	272	279	275
263	382	313	283	340	366	192	349	349	293	354
258	271	269	316	234	281	341	304	363	211	418
136	367	157	343	318	37	405	401	320	224	149
322	0	373	305	348	395	240	326	348	333	202
277	51	403	409	181	373	282	290	342	348	356
286	352	273	289	397	295	391	247	282	346	289
143	384	380	184	271	348	295	353	225	193	454
214	323	285	242	310	120	283	280	308	211	287
0	301	179	304	373	336	325	191	330	266	360
296	332	303	328	323	277	302	292	262	337	310
316	114	238	399	334	339	232	361	327	271	298
221	266	274	284	319	282	258	277	306	248	364
268	306	356	301	336	276	380	324	315	335	392
266	295	164	252	322	247	262	200	327	297	327
386	288	257	327	274	315	228	303	270	271	

266

1530.9_1185EK13	271	256	278	298	274	248	269	249	374	266
	279	245	293	393	330	327	307	272	396	263
	285	211	372	263	327	300	310	258	305	286
	303	303	324	311	336	304	400	309	213	276
	999	306	385	246	214	460	474	194	224	265
	252	231	241	222	241	276	219	243	297	197
	246	313	262	253	246	210	253	256	295	265
	250	221	287	256	251	305	197	266	298	313
	292	323	288	240	306	193	333	276	342	240
	253	316	301	254	245	203	270	204	549	250
	265	278	280	281	255	225	227	268	227	263
	195	255	179	279	288	257	156	177	193	260
	236	206	252	231	243	271	224	248	230	169
	211	348	235	221	266	261	243	285	286	329
	238	233	266	258	238	249	254	217	269	257
	272	211	217	208	262	231	202	171	160	152
	198	220	185	167	230	182	249	232	213	214
	316	250	147	242	264	269	389	261	273	277
	308	300	291	272	326	305	199	315	312	191
	264	280	259	308	244	302	343	238	342	237
	135	359	228	358	285	74	974	354	353	182
	292	0	354	240	297	458	244	272	324	279
	287	93	301	271	204	290	350	308	336	323
	202	372	229	264	311	279	292	195	278	605
	151	361	271	263	236	296	266	302	245	258
	206	331	311	214	402	187	328	277	268	125
	0	231	154	304	514	390	322	235	318	236
	280	324	286	305	254	253	328	248	213	284
	252	73	262	327	257	305	240	352	312	255
	191	243	277	282	247	246	178	271	205	276
	305	229	264	422	440	268	326	251	212	303
	274	249	109	274	226	227	257	109	269	294
	254	223	273	290	263	277	207	254	197	256

267

1533.6_1344EC21	348	346	243	384	378	336	375	207	342	350
368	383	679	435	319	361	359	292	349	410	367
417	261	368	566	301	310	608	388	340	386	329
354	355	299	297	326	225	341	415	368	362	331
306	999	335	280	166	351	445	256	382	660	358
336	329	311	320	347	319	316	357	292	308	334
340	319	328	338	327	295	667	305	229	262	328
252	276	608	284	278	357	184	357	319	352	320
315	329	326	350	333	213	322	307	315	315	339
321	316	274	187	302	192	301	658	548	345	344
253	295	292	297	343	310	218	360	267	364	331
293	313	180	312	293	294	211	677	293	407	303
289	318	321	251	326	473	184	292	273	249	201
251	490	281	306	305	304	269	306	318	352	294
276	300	311	324	311	289	316	266	306	311	314
308	173	177	289	321	308	201	258	102	254	277
260	250	264	251	173	263	320	280	281	172	379
375	310	50	701	297	375	357	203	242	390	236
635	334	276	244	326	363	252	364	401	259	323
323	485	345	372	314	310	445	470	349	220	309
283	355	185	265	373	222	314	462	344	317	173
308	0	299	349	383	436	356	431	369	342	175
229	137	331	269	365	342	269	361	363	331	340
219	312	386	300	288	616	334	425	338	349	342
525	319	331	299	286	283	527	332	214	149	376
209	318	320	176	606	252	345	243	312	82	367
0	292	140	255	547	261	279	196	323	354	357
291	374	664	307	292	239	466	220	672	298	348
282	37	662	337	308	448	491	574	450	237	271
159	203	458	306	325	321	268	263	299	269	346
259	297	319	347	347	329	349	293	238	311	277
311	322	145	298	287	167	328	114	331	286	319
290	276	256	274	237	301	193	273	254	230	

268

1559.6_2011EC33	365	387	0	388	407	304	346	220	646	204
366	445	382	425	505	525	324	386	481	409	343
505	262	505	311	299	444	453	376	635	430	624
641	645	441	497	648	0	586	333	421	381	335
385	335	999	458	213	418	376	259	410	335	682
376	538	535	541	365	288	529	289	590	282	440
257	617	468	453	245	361	360	453	417	351	347
304	421	350	400	451	431	215	386	422	510	537
546	490	551	367	544	129	549	546	525	674	504
676	533	545	164	539	150	554	301	377	637	642
337	571	558	568	402	429	281	513	338	518	613
492	249	234	726	672	534	260	298	368	342	436
309	380	264	318	353	181	137	337	283	314	156
321	234	318	374	352	313	324	399	397	421	397
325	433	418	507	509	392	497	410	564	501	569
408	0	264	528	473	490	229	379	110	389	387
341	337	357	376	0	250	242	443	429	0	385
444	450	9	268	312	346	648	226	177	496	29
343	428	714	247	461	353	315	443	478	549	294
347	14	353	425	323	530	357	314	448	300	511
325	658	171	281	363	8	391	306	889	473	199
445	0	399	287	325	284	386	381	593	538	0
248	72	328	535	236	593	155	383	551	647	474
346	424	385	279	386	255	326	74	489	340	759
159	467	552	464	447	284	205	403	101	125	526
292	548	505	285	274	331	550	334	545	38	575
15	512	23	513	304	433	606	269	604	403	572
471	712	272	558	325	249	141	266	309	556	489
355	205	422	545	542	618	302	508	541	314	224
227	249	503	494	509	442	321	335	464	371	582
381	303	439	450	440	387	416	452	334	524	387
423	380	213	391	456	77	455	234	476	474	455
249	409	245	259	270	249	233	287	193	260	

269

1560.6_1164EK04	275	261	258	409	332	299	331	166	403	306
224	307	279	363	268	346	324	241	317	342	537
507	216	351	378	260	278	309	569	312	521	301
305	305	292	317	368	212	333	345	429	306	197
246	280	458	999	128	286	287	289	243	271	276
560	300	312	296	336	393	294	234	347	223	269
237	340	240	269	205	248	246	258	279	251	291
277	328	251	250	267	293	248	215	276	287	298
310	291	325	307	302	225	338	353	325	353	287
358	307	320	187	315	185	324	265	308	362	365
235	305	306	331	680	229	183	275	263	272	274
211	196	166	288	288	229	224	253	256	312	259
269	298	268	264	289	256	183	479	264	305	161
289	304	248	276	247	233	251	282	282	301	244
248	277	223	338	341	275	324	269	358	347	340
277	181	173	313	318	338	180	255	71	255	258
248	139	258	242	173	182	263	289	252	191	367
347	332	55	183	346	331	402	168	257	341	115
325	309	340	188	271	322	414	302	509	219	227
321	159	288	286	443	281	306	350	332	169	324
192	329	233	190	388	70	188	222	366	900	146
240	0	256	221	300	271	546	268	345	332	133
151	48	417	271	244	359	193	350	319	360	382
295	252	235	214	221	252	247	228	366	286	266
142	266	298	261	285	305	251	284	208	78	415
139	334	271	187	246	314	300	245	337	106	366
8	271	69	282	256	323	309	351	321	670	373
309	309	238	508	257	199	219	220	275	504	237
312	225	152	300	310	340	176	278	355	239	245
256	220	315	294	284	280	236	261	281	232	272
294	238	277	295	265	297	303	285	136	295	237
267	250	109	313	268	104	316	156	303	310	300
163	214	211	238	215	272	178	235	192	210	

270

1565.2_1164EK04	232	359	30	235	213	258	187	170	216	91
212	306	166	202	214	257	146	186	240	227	141
210	248	228	174	220	219	185	234	240	242	215
241	248	195	164	183	172	195	221	204	244	195
214	166	213	128	999	207	230	254	261	194	200
320	223	190	205	261	195	192	168	184	192	189
173	199	227	197	171	179	176	206	230	190	228
194	270	212	176	230	203	222	198	273	236	204
219	219	192	142	220	131	196	218	197	186	211
187	199	210	135	206	110	237	217	195	219	215
213	179	178	180	249	174	306	220	226	221	187
182	220	200	213	191	161	236	187	205	178	161
258	287	200	175	209	197	173	195	223	183	111
219	175	185	196	174	191	182	221	200	227	219
215	192	231	197	190	180	203	178	210	216	204
200	118	110	185	211	208	182	246	7	242	248
57	11	188	221	20	116	252	211	195	30	245
165	170	180	122	224	187	198	187	49	315	3
99	201	219	82	144	140	207	139	196	77	323
143	197	265	285	226	182	180	186	109	0	120
250	174	49	138	178	164	182	225	223	99	929
172	0	236	163	216	167	290	174	216	200	0
227	160	206	145	119	189	110	157	222	209	235
60	112	139	156	145	207	126	0	155	172	209
194	201	256	5	131	127	166	146	146	0	193
146	98	248	134	208	82	222	172	212	51	178
317	153	182	168	161	218	194	56	208	231	240
207	220	170	248	150	181	195	150	180	177	110
60	2	159	189	193	227	212	227	237	181	134
91	142	200	208	234	198	162	126	116	192	185
129	155	199	209	207	168	214	169	8	114	211
174	203	19	223	172	59	180	88	229	203	219
152	135	221	192	176	239	188	219	241	166	

271

1608.3_2011EC27	302	315	213	311	276	331	299	311	435	287
254	246	377	388	418	477	267	359	374	319	370
365	220	402	348	325	458	348	326	368	358	397
378	362	424	437	397	254	441	386	326	343	327
460	351	418	286	207	999	428	327	306	322	387
303	297	316	309	320	281	295	346	319	369	281
341	366	350	285	368	338	273	326	459	358	430
340	332	313	367	378	440	285	351	289	388	275
301	390	342	364	354	234	347	417	346	358	386
379	333	325	263	342	222	350	232	433	373	377
320	307	308	322	300	252	319	324	302	322	376
267	353	171	335	337	305	303	257	359	391	312
359	340	276	175	321	369	218	321	371	320	208
329	361	342	326	328	329	325	344	336	396	338
314	290	353	348	341	302	346	322	330	360	360
350	214	228	350	339	330	219	236	181	233	233
304	232	250	186	299	221	392	280	317	236	304
380	456	211	280	313	299	428	298	282	288	141
351	466	377	370	451	345	373	388	399	283	285
316	307	343	372	250	368	348	320	488	219	442
208	397	213	339	366	110	429	333	403	306	236
380	136	434	347	370	391	340	389	390	344	371
361	191	327	426	440	408	363	383	389	354	393
397	469	338	344	315	343	372	342	349	453	358
185	457	285	311	318	322	274	345	393	239	504
359	378	379	229	344	255	357	269	335	261	339
232	281	251	320	411	464	343	319	354	358	370
371	368	298	369	338	344	365	262	264	403	346
346	241	330	381	312	381	231	380	411	367	339
333	261	404	353	356	350	315	318	283	330	413
347	321	346	476	461	298	445	357	306	445	379
330	309	231	314	365	189	386	242	361	366	339
322	345	455	492	396	457	335	453	420	294	

272

1627.1_1185EK12	324	293	237	389	325	319	370	266	389	359
259	329	393	420	344	418	369	364	304	386	422
404	210	340	408	308	374	391	356	345	468	378
332	331	398	420	332	231	372	372	320	397	432
474	445	376	287	230	428	999	213	264	339	343
350	283	284	284	392	313	277	280	301	237	247
289	277	275	255	256	273	323	275	274	325	419
257	315	356	325	296	332	204	326	268	335	251
268	289	283	329	284	220	339	374	345	350	282
354	340	332	237	334	199	331	276	505	368	364
276	269	270	289	334	250	303	248	262	243	316
252	275	263	297	295	276	282	240	237	342	264
274	308	280	271	474	363	209	457	328	226	186
292	359	287	281	309	304	271	319	323	359	276
343	265	342	354	347	351	337	238	345	350	328
350	187	232	317	349	333	184	253	129	262	267
280	278	217	268	206	229	321	288	295	161	360
366	282	126	323	327	370	440	242	328	325	162
352	443	356	254	434	338	410	360	436	223	342
316	296	314	372	418	333	449	393	454	195	424
390	348	240	368	368	208	478	437	379	323	174
266	0	359	295	358	927	376	320	351	293	44
297	92	362	440	271	369	275	395	397	330	371
340	399	269	309	270	343	352	270	288	476	255
242	346	380	241	281	279	306	373	248	207	491
254	355	379	254	424	307	291	257	279	189	348
9	310	182	322	493	389	296	235	308	359	388
340	309	337	329	240	281	349	246	321	396	265
330	137	301	343	268	360	280	406	327	320	304
248	238	423	386	337	305	285	319	249	305	397
365	319	296	403	430	267	423	299	253	313	328
267	271	116	321	304	185	383	213	349	352	336
254	270	304	343	325	331	265	320	301	280	

273

1628.2_1344EC22	298	308	189	246	235	255	252	232	255	160
208	244	250	298	239	215	205	216	226	278	249
297	214	306	276	194	269	288	268	264	273	227
259	242	206	293	267	202	245	271	308	261	204
194	256	259	289	254	327	213	999	239	271	254
348	225	206	218	266	251	204	304	210	223	230
302	218	263	225	228	312	254	233	210	211	245
225	221	255	218	277	324	609	197	275	265	243
248	226	218	174	237	261	206	257	202	245	225
257	193	190	174	197	306	215	251	282	285	299
252	199	197	211	287	200	223	231	284	228	159
208	235	224	197	174	212	289	233	358	286	253
265	335	269	258	206	249	175	238	249	217	176
300	247	222	278	249	266	251	303	295	332	246
215	208	180	222	215	281	213	194	248	252	248
302	176	234	239	217	215	276	195	78	253	218
184	128	233	211	156	114	347	262	226	185	220
262	322	239	197	243	252	272	218	123	286	147
232	101	282	154	223	186	204	317	307	200	284
203	243	252	306	246	223	236	302	200	147	292
183	290	103	166	301	167	176	230	255	266	255
290	215	252	137	266	193	337	226	231	222	136
253	123	265	252	241	268	213	249	242	226	336
238	125	194	203	227	296	211	174	193	244	168
192	305	193	199	236	194	221	197	306	72	331
163	209	250	259	253	139	225	196	220	219	244
159	197	253	214	264	268	212	184	213	286	241
213	228	265	240	185	300	215	270	302	241	231
255	69	190	249	198	226	223	218	223	303	265
189	267	265	307	240	204	212	199	215	229	179
160	169	199	272	259	267	337	253	201	230	200
184	251	105	230	243	154	214	221	232	208	219
184	156	320	290	276	351	327	310	308	227	

274

1630.2_1135EC00	330	287	190	328	318	349	255	207	383	200
193	424	352	333	238	293	223	219	304	391	246
362	244	413	367	267	362	364	298	367	334	393
355	376	264	304	318	244	341	419	280	305	196
224	382	410	243	261	306	264	239	999	333	345
278	350	353	349	257	288	348	289	301	281	322
269	263	355	320	274	285	346	317	236	287	298
285	278	323	268	254	321	237	202	256	310	284
296	308	346	290	319	139	276	297	283	255	298
277	264	256	241	276	189	279	337	326	296	303
270	264	262	282	267	303	305	260	296	267	244
245	255	196	264	255	283	262	353	233	351	262
287	338	256	240	327	377	188	288	301	290	212
285	403	213	259	209	226	218	254	267	338	214
246	280	261	300	299	226	306	251	277	293	318
258	186	287	264	317	292	196	207	206	182	217
267	265	186	219	232	223	337	170	269	199	376
283	235	159	319	321	255	394	240	195	449	146
301	241	330	263	276	409	231	379	392	218	409
407	311	402	481	288	366	347	323	285	38	319
274	316	233	228	325	203	250	348	325	257	238
333	237	296	184	356	286	336	284	321	328	178
332	94	301	320	265	371	260	397	383	330	338
208	282	308	314	249	355	349	290	279	302	258
233	286	322	257	228	272	303	253	301	217	380
265	264	316	264	335	233	310	196	371	231	291
2	272	209	278	320	305	243	265	266	343	337
219	261	359	252	304	335	293	288	305	316	215
327	158	338	387	285	341	274	346	379	344	350
207	292	325	271	243	235	286	258	231	227	349
270	221	327	297	328	257	438	279	218	315	298
255	266	190	271	296	177	283	260	305	328	269
257	304	349	373	345	343	269	331	327	322	

275

1636.7_1135ec00	333	313	210	338	328	345	348	174	327	245
290	278	695	365	240	336	319	221	260	361	370
381	210	316	587	295	358	594	401	325	380	296
334	314	236	270	299	215	323	445	302	374	268
265	660	335	271	194	322	339	271	333	999	261
342	263	270	268	372	285	262	328	284	251	264
332	297	263	273	291	262	788	271	225	257	348
231	292	566	264	246	308	189	354	255	292	230
234	255	253	329	262	238	318	346	311	298	250
298	291	268	195	292	170	283	712	633	313	300
237	254	254	258	323	275	240	276	245	276	252
232	266	157	271	276	262	247	766	274	392	280
289	306	262	190	302	580	180	286	325	313	217
273	545	242	258	282	280	272	294	321	318	282
250	279	256	290	282	262	277	233	269	281	269
284	162	218	272	287	283	234	196	135	234	234
237	176	229	245	180	193	245	254	226	174	308
359	317	87	774	334	348	344	164	193	321	103
732	326	257	243	270	315	253	341	399	227	351
334	594	328	377	312	314	444	413	234	139	285
270	326	214	223	346	213	261	522	306	310	199
215	0	249	236	344	355	303	445	302	294	155
255	102	339	242	345	305	311	362	307	316	328
223	275	332	308	227	642	288	492	287	352	275
613	282	289	244	296	271	500	283	232	160	342
200	304	292	231	715	152	283	232	258	29	343
1	227	141	284	635	248	284	222	297	308	323
311	324	729	328	220	242	410	259	721	320	310
313	31	810	309	264	412	591	551	463	240	288
251	246	416	208	330	247	183	214	274	242	319
231	263	283	314	316	287	382	266	199	292	236
288	267	115	251	248	195	324	84	310	328	303
233	210	253	269	236	303	232	269	258	222	

276

1639.3_1135EC00	343	356	123	330	337	297	317	262	478	226
299	424	317	402	505	435	292	318	452	429	356
441	267	446	297	261	397	359	306	444	358	455
450	450	430	544	552	142	519	327	368	314	332
285	358	682	276	200	387	343	254	345	261	999
310	469	453	460	328	335	456	300	491	245	417
252	517	426	425	244	348	270	414	362	313	277
342	391	302	360	476	423	197	347	389	463	477
480	447	492	336	477	218	455	446	461	614	450
616	453	436	183	462	179	444	252	308	617	620
366	457	453	478	303	492	227	409	401	411	588
576	247	309	685	634	654	277	256	334	404	471
369	325	260	387	330	165	175	343	293	246	195
332	191	331	346	362	337	317	384	362	418	397
349	443	315	497	493	399	464	485	489	457	490
417	153	215	469	450	450	189	447	228	435	456
401	357	412	442	200	323	305	501	429	167	337
575	414	93	269	284	317	482	256	198	463	138
294	407	731	257	416	346	356	428	452	581	279
323	127	300	370	268	425	273	292	422	229	551
218	558	123	342	322	120	312	281	637	291	200
463	0	384	265	306	262	332	352	479	515	21
184	103	345	438	255	480	159	339	447	510	431
280	367	232	296	337	246	321	129	396	264	721
149	397	532	313	467	316	209	394	180	89	511
272	506	405	222	221	344	493	261	448	219	414
342	384	120	404	242	460	483	214	482	333	496
452	680	227	429	323	225	178	236	267	423	533
357	76	354	412	402	450	229	432	442	240	227
208	230	439	408	425	376	274	330	421	344	458
341	317	417	381	369	343	404	469	294	469	364
467	354	195	436	511	196	389	165	456	432	469
247	374	255	262	279	327	265	339	268	231	

277

1641.7_1164EK04	315	376	219	452	344	345	385	213	422	339
229	367	314	387	289	336	364	256	293	355	499
490	214	421	360	261	293	370	635	359	561	344
349	343	282	340	357	199	335	343	437	395	210
252	336	376	560	320	303	350	348	278	342	310
999	343	331	337	371	325	320	248	346	265	317
277	360	330	319	240	299	312	320	258	298	314
253	325	326	231	371	286	364	262	295	320	316
343	328	329	269	328	231	324	351	345	337	325
334	330	327	194	348	351	348	289	342	328	326
303	301	303	326	770	274	235	262	318	260	268
239	217	258	314	293	238	347	288	350	307	285
342	311	248	297	329	265	186	525	246	328	170
356	287	263	281	277	240	263	276	261	304	236
273	288	248	348	347	335	342	314	333	342	326
290	162	218	304	357	357	214	259	74	269	270
277	166	260	245	159	221	358	285	264	157	447
353	341	176	280	348	385	428	224	277	407	111
346	239	324	234	281	280	466	290	538	189	274
324	226	339	394	537	302	291	381	310	173	292
224	322	248	165	407	157	248	248	304	552	313
229	3	248	158	368	332	969	285	339	385	46
237	75	370	271	278	339	191	337	327	355	340
198	255	217	256	270	309	305	131	359	281	278
234	329	326	228	353	311	310	252	251	99	432
133	370	347	240	309	208	333	274	332	238	293
141	300	251	290	340	326	310	299	328	722	367
362	315	286	381	338	275	252	248	312	392	276
326	137	264	301	286	356	274	341	347	283	312
253	247	345	315	346	299	226	219	285	232	260
242	231	307	292	278	281	373	321	224	286	236
282	271	76	344	313	125	380	227	339	350	341
196	237	290	268	285	315	322	309	303	265	

278

1652.8_1288EC27	278	271	198	313	289	312	305	209	551	219
259	293	318	363	334	392	298	344	341	339	302
403	236	409	309	265	363	350	313	490	441	455
485	470	368	510	742	261	672	382	334	266	318
231	329	538	300	223	297	283	225	350	263	469
343	999	967	978	297	289	975	296	792	265	480
293	776	504	481	262	334	262	515	303	334	281
349	374	258	343	335	346	216	351	435	643	887
882	692	885	223	841	154	609	522	650	684	668
709	604	630	224	651	188	640	249	257	641	643
303	617	631	746	337	470	210	420	319	422	499
449	188	309	580	588	443	290	267	306	397	582
351	361	199	335	285	266	203	354	230	248	187
322	247	380	452	420	395	388	447	398	430	392
413	539	410	573	584	413	564	489	692	588	702
432	227	297	561	571	593	212	392	274	481	406
451	416	433	478	228	318	359	493	471	256	318
395	329	134	254	305	305	594	229	201	312	144
311	343	500	252	359	333	291	390	407	257	288
311	256	302	395	372	328	293	299	265	140	524
173	702	136	205	290	115	209	216	484	310	256
345	1	392	232	291	233	362	302	545	931	29
300	164	343	350	289	660	243	404	561	800	509
288	299	227	250	395	229	348	179	574	288	651
225	550	584	417	480	251	247	285	264	214	585
175	577	609	299	215	265	921	388	864	176	573
356	528	154	566	250	370	661	171	704	348	661
535	586	247	527	288	300	277	318	233	504	598
453	201	318	529	561	597	403	468	632	324	341
209	305	626	443	515	498	289	370	609	382	569
327	317	564	536	512	474	428	572	307	502	410
506	419	171	458	533	150	526	244	580	586	504
249	407	304	389	296	364	285	381	322	324	

279

1660.4_1288EC27	307	277	200	332	310	321	327	218	535	253
281	299	305	365	329	390	323	327	326	355	324
396	241	415	313	264	376	355	329	495	441	457
489	466	383	528	748	261	682	393	348	268	321
241	311	535	312	190	316	284	206	353	270	453
331	967	999	984	344	274	981	309	793	266	486
309	779	515	483	265	345	264	515	307	361	293
361	396	292	375	355	394	179	353	458	642	898
894	693	911	249	872	161	616	521	654	699	672
713	622	636	203	668	154	643	237	262	652	654
302	650	667	757	353	490	223	429	301	427	480
539	224	303	572	567	431	273	226	332	406	575
335	353	224	355	314	272	179	350	247	250	189
304	260	418	499	458	444	438	494	423	449	418
461	524	392	572	581	404	543	480	706	566	693
387	197	285	545	559	575	202	404	288	477	414
465	417	440	481	201	309	337	511	462	207	334
392	359	134	232	308	327	570	220	206	323	152
300	349	502	252	322	339	317	417	396	236	277
317	255	330	404	377	330	288	310	276	202	536
205	687	147	197	295	69	214	226	461	320	240
349	0	399	260	331	239	349	318	544	949	27
296	169	337	345	326	664	229	387	552	793	525
281	303	249	253	416	243	363	167	578	282	647
198	564	579	424	472	269	248	352	235	161	584
256	571	582	284	219	368	933	385	889	173	540
350	550	172	583	252	387	664	194	703	357	645
527	590	250	510	239	283	276	301	232	493	593
470	243	285	545	590	621	383	463	637	300	307
210	282	640	450	514	555	319	406	599	422	580
362	356	557	549	527	503	404	560	280	492	400
489	462	201	437	528	180	495	196	558	557	472
266	413	275	358	272	337	222	354	299	341	

280

1666.9_1288EC25	290	266	201	311	287	313	315	198	545	227
266	291	300	367	330	393	307	328	330	358	328
389	248	425	299	273	379	357	312	502	444	465
496	471	386	531	751	250	676	388	360	263	318
222	320	541	296	205	309	284	218	349	268	460
337	978	984	999	312	290	982	301	816	253	480
301	782	513	474	255	335	258	511	306	348	295
359	395	284	380	347	395	181	342	463	637	902
897	691	909	239	869	144	619	518	653	700	669
718	617	633	206	664	133	642	243	256	688	690
292	654	670	756	353	484	220	432	304	431	484
522	210	316	576	573	435	271	252	315	406	579
327	351	209	346	296	278	183	343	237	265	182
304	257	402	491	444	430	425	484	410	446	408
458	543	394	587	597	393	561	491	710	581	706
384	205	298	561	571	588	225	393	292	467	406
452	400	427	470	208	313	338	508	473	215	311
387	365	111	243	301	315	582	212	207	313	150
312	353	503	228	328	350	291	408	399	240	277
310	268	312	399	380	332	274	297	280	192	542
202	694	147	208	312	58	192	223	466	305	235
354	0	401	234	315	240	344	314	549	947	29
290	166	348	348	290	682	238	400	561	796	541
277	298	230	237	423	236	361	179	572	288	659
216	569	569	447	474	263	253	350	196	162	590
221	573	594	297	212	329	936	385	893	173	542
401	547	173	585	245	390	667	168	709	358	645
531	596	243	515	236	282	265	316	228	498	592
469	246	298	547	594	620	406	469	642	292	325
229	304	637	445	514	540	307	392	593	408	580
364	355	551	553	530	501	403	578	293	492	406
498	454	195	439	536	182	504	208	572	573	486
252	416	268	364	266	330	214	343	284	346	

1674.4_1164EK04	323	310	212	352	312	280	278	169	335	240
235	340	319	369	282	423	286	222	310	384	290
529	169	367	353	287	360	375	428	309	557	347
320	312	311	361	295	200	309	316	377	516	226
241	347	365	336	261	320	392	266	257	372	328
371	297	344	312	999	324	307	262	326	218	301
239	303	312	302	270	262	327	295	260	253	318
224	290	375	212	314	294	205	259	251	300	244
254	289	296	329	280	268	298	297	292	286	279
279	279	248	189	246	201	264	247	393	298	300
250	253	254	296	335	258	221	248	331	247	264
230	328	231	283	294	239	271	253	207	338	228
309	341	268	252	555	340	198	475	364	343	194
298	332	255	257	261	275	241	280	256	318	247
230	238	305	269	264	229	276	232	264	277	270
196	191	226	210	291	278	216	224	82	220	229
213	108	206	192	174	197	327	267	245	157	327
368	297	133	377	323	278	352	221	275	355	111
337	392	334	258	309	359	205	372	536	234	329
310	309	385	368	488	305	467	341	317	134	334
471	274	280	278	400	292	198	252	315	352	180
245	0	236	161	365	376	426	284	297	368	160
503	153	362	342	281	303	264	379	336	347	307
279	304	309	232	213	335	310	275	280	346	248
245	280	307	264	227	334	299	354	238	163	408
184	272	305	224	357	205	275	205	280	229	254
4	271	250	296	407	324	288	147	294	419	334
252	277	320	310	304	263	303	257	310	288	245
318	160	315	316	243	295	300	363	348	271	290
317	255	298	337	264	246	237	273	233	264	282
288	275	279	282	271	271	378	268	171	300	202
263	236	102	240	261	94	259	256	290	307	257
280	245	289	286	271	326	298	310	291	215	

282

1681.2_1164EK04	549	328	159	379	314	626	346	229	356	300
305	387	349	418	259	344	330	228	294	514	499
406	268	306	586	248	337	365	369	299	360	297
297	312	339	320	386	106	379	500	464	326	367
276	319	288	393	195	281	313	251	288	285	335
325	289	274	290	324	999	275	266	285	214	337
272	307	346	352	243	307	308	343	309	280	356
247	322	370	273	258	362	182	318	301	291	319
321	278	336	563	327	212	303	387	289	348	268
351	286	285	139	305	203	293	274	345	379	371
202	277	286	306	350	305	303	277	211	274	277
271	290	125	288	284	266	190	229	290	432	276
241	347	302	215	328	391	137	322	392	372	152
213	396	252	302	258	256	257	306	284	305	282
238	260	312	347	338	304	312	269	313	296	312
292	142	288	311	323	326	220	250	86	264	259
215	246	275	231	155	168	316	239	265	147	340
394	388	31	304	616	346	371	156	223	385	183
290	328	310	173	280	451	385	397	360	278	379
487	219	422	418	264	251	465	459	318	197	333
279	359	294	342	496	0	261	291	311	385	176
318	0	348	287	450	283	353	313	320	318	109
212	89	960	364	311	330	203	302	323	319	403
214	236	210	312	414	328	284	217	290	329	322
170	433	400	137	301	256	307	328	218	185	482
248	317	287	286	294	188	312	283	306	60	325
9	216	85	258	307	299	313	185	327	333	354
311	310	319	320	366	296	292	305	328	341	286
241	27	256	308	278	347	241	355	352	274	283
346	306	383	301	331	293	199	230	250	232	369
265	221	353	331	320	285	346	324	187	267	303
298	256	101	285	313	149	319	135	364	314	323
317	259	302	312	256	300	189	309	285	188	

283

1681.9_1288EC26	284	263	199	313	291	303	316	200	529	234
264	283	311	365	329	390	310	329	326	348	309
380	236	414	306	257	377	366	309	491	435	458
487	467	380	531	744	275	678	385	345	252	310
219	316	529	294	192	295	277	204	348	262	456
320	975	981	982	307	275	999	303	788	252	473
303	773	505	467	257	329	257	504	308	347	291
359	389	283	385	352	390	183	337	452	633	888
883	687	900	226	858	149	608	517	643	692	664
709	606	624	214	651	166	633	241	255	648	649
282	615	632	752	350	479	211	421	298	424	480
521	212	296	567	563	429	272	246	317	403	574
329	355	209	329	303	277	186	344	230	258	183
300	262	402	492	443	427	424	481	407	445	406
457	519	378	565	574	389	535	471	701	564	687
373	205	287	542	552	572	214	389	284	461	402
447	398	424	467	210	311	341	506	458	217	317
393	365	114	242	291	316	567	213	211	304	154
322	354	513	245	327	331	287	404	391	232	284
316	267	307	392	372	328	280	293	271	165	545
184	697	151	195	297	60	189	220	460	304	219
353	0	399	244	321	235	337	307	555	932	27
302	165	339	342	321	660	227	383	553	788	522
274	322	220	244	419	239	363	175	576	278	646
218	565	566	418	468	269	253	343	250	151	578
223	566	579	286	214	350	924	385	884	183	533
388	529	181	562	247	381	658	167	697	353	638
524	584	248	509	239	284	276	305	227	495	585
466	244	294	528	558	604	401	462	641	294	326
226	295	629	444	502	539	312	388	584	406	574
356	354	553	549	525	501	404	557	276	491	398
475	445	190	435	520	168	501	210	551	553	469
266	407	275	362	275	335	222	345	285	347	

1708.9_1344EC71	223	252	193	217	279	231	267	651	371	274
286	254	355	345	286	275	241	344	281	303	195
309	220	329	319	279	329	343	244	309	313	314
305	305	285	305	355	214	378	301	259	282	266
243	357	289	234	168	346	280	304	289	328	300
248	296	309	301	262	266	303	999	327	765	202
924	337	250	206	746	634	304	235	369	707	281
613	283	305	358	265	402	278	282	282	335	312
321	289	320	202	336	219	303	360	297	334	299
327	285	255	233	258	252	258	303	290	320	320
316	292	297	328	215	306	213	327	289	322	300
287	249	198	337	333	289	364	336	330	364	317
320	304	242	250	241	315	166	281	216	209	203
372	263	490	542	497	499	497	540	509	572	510
513	296	312	308	313	277	322	296	320	330	322
295	161	188	287	332	318	288	276	206	309	287
300	213	248	299	260	259	370	320	324	189	256
284	319	232	303	224	267	357	655	203	244	187
336	214	264	312	339	286	166	297	326	302	288
246	264	253	311	270	317	346	340	308	146	325
243	362	247	221	276	175	234	288	300	208	125
300	157	307	281	312	269	253	370	286	317	133
305	353	288	272	289	359	258	327	308	327	560
328	267	343	269	314	308	717	293	281	289	307
249	369	333	254	273	669	310	319	346	201	369
304	332	318	261	285	311	315	269	326	247	298
182	275	197	307	301	369	305	223	318	240	327
316	339	316	329	590	287	304	278	330	323	342
500	458	297	341	294	348	265	346	392	314	295
181	320	370	326	296	583	402	508	288	532	361
418	509	333	324	329	565	439	347	252	335	522
310	543	471	293	322	143	332	230	326	337	269
464	431	470	510	434	500	352	457	460	347	

285

1710.0_1288EC37	291	249	8	333	318	273	354	251	647	247
252	327	276	315	350	421	295	329	339	357	381
457	229	468	261	218	398	294	354	502	447	484
487	485	431	483	827	6	713	356	358	297	346
297	292	590	347	184	319	301	210	301	284	491
346	792	793	816	326	285	788	327	999	268	471
333	930	474	472	266	420	264	475	325	399	283
380	422	245	407	346	450	197	412	469	648	834
819	684	803	286	822	112	724	631	743	803	663
802	724	748	32	761	152	751	231	255	768	770
342	750	767	874	363	473	260	502	345	509	554
466	260	303	688	652	434	282	220	326	372	620
338	331	274	340	294	151	32	373	289	288	198
302	167	462	522	474	451	469	512	453	461	465
486	646	428	653	669	443	640	565	763	649	743
457	10	299	654	611	619	209	436	309	478	448
422	410	479	509	9	308	309	510	546	12	358
331	384	139	203	257	354	667	217	176	321	100
283	418	488	159	333	332	390	395	441	275	251
254	133	239	357	352	333	264	275	306	189	506
243	738	248	238	280	58	297	254	560	327	226
382	0	415	240	332	260	362	309	609	780	44
206	164	348	376	270	800	181	448	618	942	578
307	411	319	208	407	199	351	109	685	269	685
162	550	706	514	565	262	228	402	167	192	648
247	668	654	284	199	239	850	437	846	113	666
415	625	118	664	278	425	823	219	840	396	743
625	685	172	647	350	247	149	307	248	620	636
485	243	335	661	701	725	453	532	682	280	263
190	300	680	556	612	631	333	451	648	464	550
435	363	608	618	605	520	429	665	333	498	460
568	489	202	420	615	176	591	155	619	629	601
318	445	258	319	280	293	221	330	257	294	

286

1719.5_1344EC71	249	245	209	226	249	222	285	578	329	217
289	239	288	324	278	310	255	304	219	299	223
274	224	311	287	290	297	282	241	317	290	311
313	322	252	306	297	209	303	273	218	232	254
197	308	282	223	192	369	237	223	281	251	245
265	265	266	253	218	214	252	765	268	999	266
803	270	293	262	853	622	269	240	371	674	241
650	290	280	297	244	384	197	293	285	301	264
277	265	253	170	277	175	299	307	288	307	259
299	276	272	206	270	225	286	269	255	281	279
257	259	260	273	256	322	259	304	252	314	218
281	195	234	250	244	244	300	280	314	338	251
240	283	221	226	215	267	165	222	222	184	204
292	250	515	588	525	521	503	562	521	535	511
482	231	172	268	280	233	252	236	257	280	253
211	131	161	251	269	253	284	252	106	269	259
279	81	260	240	210	223	323	303	263	142	239
277	355	242	230	223	285	311	580	194	256	272
295	238	238	277	291	279	171	337	294	237	292
294	236	274	352	274	283	303	335	307	110	309
196	271	222	207	231	143	173	262	255	240	142
270	177	220	306	303	193	253	417	253	270	46
246	287	233	253	228	255	243	239	265	272	553
210	235	337	230	309	256	662	220	244	248	221
190	384	223	171	234	731	285	302	244	149	340
228	282	288	248	257	281	255	264	248	204	290
220	213	183	274	258	333	236	180	263	270	292
276	236	289	281	561	250	220	258	277	286	240
526	463	225	260	243	236	187	230	305	249	238
87	282	275	292	269	602	411	530	269	532	322
410	455	271	286	307	528	358	278	134	245	527
233	541	486	262	271	156	268	207	262	244	239
487	387	387	417	342	382	327	367	348	244	

287

1722.2_1288EC39	363	273	193	243	260	323	275	210	533	162
245	503	309	363	312	347	278	283	294	336	363
481	296	639	337	259	400	347	323	561	331	531
576	565	360	381	516	245	488	367	390	304	272
248	334	440	269	189	281	247	230	322	264	417
317	480	486	480	301	337	473	202	471	266	999
239	475	946	969	258	280	281	931	295	297	283
275	342	288	320	363	318	166	279	359	428	424
427	425	432	291	418	171	483	455	468	439	432
434	469	462	228	466	167	458	207	243	468	456
313	418	420	443	285	437	255	438	306	430	402
404	263	313	447	439	335	256	206	256	397	369
338	327	192	355	353	267	198	352	240	258	177
277	282	331	314	333	340	310	349	323	420	301
284	349	290	505	508	252	483	378	463	462	471
235	216	451	405	488	473	228	282	203	244	294
257	332	231	300	216	270	303	339	381	230	256
361	297	171	249	295	275	537	219	197	493	149
276	341	391	240	346	331	293	603	504	329	353
416	244	506	582	256	306	301	349	355	89	410
247	555	230	227	409	21	217	203	416	320	141
334	0	355	231	347	240	328	288	506	528	27
248	130	367	429	248	462	239	319	614	481	421
280	327	253	254	344	248	343	204	372	289	416
211	427	418	304	394	291	257	393	223	245	522
237	464	461	447	213	256	448	382	426	147	418
399	430	169	434	227	339	458	154	464	293	482
425	441	238	397	286	356	227	450	257	391	384
399	190	279	384	397	408	291	393	408	356	390
222	434	414	358	425	338	286	317	360	305	550
312	263	349	384	360	319	421	421	181	374	310
405	366	207	433	404	90	449	167	513	501	382
232	361	299	340	330	358	231	359	308	307	

1723.3_1344EC71	258	242	223	209	303	234	318	617	372	316
282	239	334	317	248	272	311	323	227	318	215
316	217	327	348	265	322	349	238	308	327	288
304	311	268	284	348	225	349	297	231	270	282
246	340	257	237	173	341	289	302	269	332	252
277	293	309	301	239	272	303	924	333	803	239
999	337	268	237	787	617	286	250	336	678	308
604	268	271	348	254	387	234	269	263	318	302
319	298	309	217	329	175	309	357	301	330	282
328	290	264	259	264	225	284	311	292	306	307
303	301	305	336	228	315	227	300	270	298	268
299	225	182	318	321	279	323	325	316	332	302
297	274	227	217	233	304	191	258	218	234	201
330	274	496	546	518	515	497	554	525	530	507
484	256	298	297	306	271	293	259	317	305	310
289	174	182	261	299	294	262	258	186	286	260
310	211	245	274	266	257	357	291	284	204	263
273	312	222	274	242	318	350	624	267	255	193
308	218	242	287	328	292	179	313	304	223	326
254	249	248	310	273	291	332	334	300	141	305
277	334	251	237	263	175	230	315	246	219	133
282	156	301	277	293	260	265	370	286	322	114
305	303	284	263	301	355	288	302	296	333	554
265	266	317	257	317	277	678	300	279	297	256
243	364	290	216	254	654	267	327	339	152	375
270	325	306	256	277	294	325	290	333	204	302
177	275	183	288	298	320	282	198	313	246	332
312	333	326	302	569	268	282	255	296	307	296
506	442	282	316	286	310	245	326	384	291	286
170	299	350	268	305	575	396	499	275	531	332
400	471	289	304	314	564	396	323	221	308	484
266	528	487	281	307	190	289	212	300	303	282
445	404	444	487	396	454	335	418	421	311	

289

1726.6_1135EC25	319	291	99	338	328	299	325	232	700	237
273	353	303	351	454	491	272	336	389	352	381
471	252	517	303	226	445	316	344	589	435	545
575	563	444	520	878	120	750	365	352	286	304
313	319	617	340	199	366	277	218	263	297	517
360	776	779	782	303	307	773	337	930	270	475
337	999	513	486	266	406	288	504	386	407	281
372	485	245	415	375	458	216	419	482	680	797
791	723	812	309	789	142	756	664	778	800	684
801	752	785	107	813	179	796	231	267	786	788
347	787	801	881	370	476	236	516	338	522	556
435	262	281	706	677	418	302	205	351	376	587
351	341	279	332	296	154	122	385	269	247	210
315	186	436	495	455	427	458	481	443	464	432
458	604	407	657	676	418	650	541	740	655	725
426	120	325	670	626	633	189	437	289	443	448
402	393	450	497	135	307	312	509	535	146	377
391	394	111	194	274	325	718	215	162	374	137
277	490	526	230	371	357	399	407	475	265	293
277	145	254	382	324	402	313	300	399	143	522
242	821	249	253	308	59	317	268	584	334	210
393	0	430	284	312	216	386	311	677	772	47
220	153	352	440	268	796	196	435	621	980	592
326	391	295	242	412	235	377	113	612	275	626
165	539	700	503	555	311	195	422	185	206	643
280	695	667	328	200	287	820	397	792	152	697
410	648	127	677	247	432	845	223	860	389	727
651	697	187	664	370	280	169	362	209	639	590
437	246	387	691	721	754	466	552	687	291	261
199	342	666	566	657	591	309	422	607	492	621
459	357	589	623	617	514	496	642	306	538	436
544	451	206	469	602	185	600	176	636	635	598
310	447	266	348	292	337	235	355	266	317	

1730.5_1288EC39	352	280	204	303	311	346	279	234	565	194
304	490	301	348	354	366	266	335	307	321	333
490	274	621	324	259	408	356	333	593	340	589
608	596	384	425	534	244	485	385	408	313	316
262	328	468	240	227	350	275	263	355	263	426
330	504	515	513	312	346	505	250	474	293	946
268	513	999	936	288	265	290	948	320	286	269
276	346	290	352	380	346	215	334	378	447	434
441	452	443	211	429	193	539	473	526	480	459
476	527	514	242	510	219	511	246	247	472	458
339	473	477	476	319	475	230	491	309	484	409
417	293	346	468	463	345	291	237	287	395	386
350	375	255	390	358	282	240	349	269	297	195
330	282	327	337	352	343	339	393	338	415	314
303	370	347	508	510	309	481	381	468	480	476
298	240	435	408	513	510	258	316	200	296	321
310	325	286	307	265	293	353	371	380	298	308
376	237	197	211	320	279	581	219	143	502	137
255	346	396	244	387	306	267	590	506	256	335
432	189	517	574	285	340	306	363	367	200	452
298	590	220	200	422	109	257	201	443	304	203
351	0	372	258	325	232	344	315	539	540	29
281	109	362	436	276	453	242	313	583	520	421
309	294	205	278	386	240	358	150	388	279	415
217	465	477	266	414	247	240	403	240	191	533
250	506	526	446	215	177	451	376	425	195	461
406	484	155	493	223	347	493	178	519	310	512
463	492	229	459	284	384	237	440	301	452	395
374	52	306	448	460	454	321	390	440	396	400
230	431	417	443	461	360	278	310	402	346	545
313	308	370	409	393	358	458	429	255	381	341
392	363	162	468	396	104	486	236	507	514	394
253	361	356	383	370	387	315	391	363	302	

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1731.6_1288EC30	364	271	185	242	269	328	272	208	545	153
241	518	307	369	316	353	272	287	298	342	359
486	293	653	335	264	399	344	323	567	336	541
584	574	370	388	524	237	492	367	387	303	272
253	338	453	269	197	285	255	225	320	273	425
319	481	483	474	302	352	467	206	472	262	969
237	486	936	999	251	281	288	948	298	300	288
274	346	271	311	367	324	174	286	366	437	430
435	434	439	293	428	178	483	462	469	445	442
440	469	456	247	467	167	453	211	243	474	461
321	424	428	459	291	427	251	447	315	441	400
406	240	318	457	442	341	258	212	252	406	379
342	333	195	367	352	260	215	347	254	274	179
277	280	328	322	331	337	310	349	321	420	308
288	356	299	510	514	263	493	388	477	485	486
241	235	459	435	517	497	230	294	211	249	306
264	350	237	314	235	266	304	352	391	253	258
368	300	174	248	303	272	548	218	192	507	143
276	349	394	242	347	336	288	610	508	338	356
393	247	489	567	257	311	304	347	373	93	421
246	573	229	229	401	21	216	204	423	317	150
352	0	362	231	349	239	329	305	518	531	27
249	127	376	435	253	471	243	326	624	488	429
279	287	252	253	360	251	349	214	378	289	422
203	440	420	306	413	295	245	394	207	248	539
240	480	469	453	214	251	454	382	432	157	428
393	429	165	432	228	342	464	161	467	298	481
440	449	235	404	280	361	228	456	261	401	410
403	188	284	388	405	418	298	390	415	363	399
228	438	422	355	436	340	282	309	366	299	556
321	267	355	389	365	318	431	436	191	378	315
413	369	209	432	429	86	455	166	526	512	393
237	368	311	345	335	362	233	362	309	305	

1731.7_1344EC71	211	230	206	254	265	207	306	570	309	275
313	261	302	316	249	259	281	286	196	308	208
297	211	302	299	281	289	301	246	300	303	277
314	315	242	296	288	195	288	278	240	277	280
246	327	245	205	171	368	256	228	274	291	244
240	262	265	255	270	243	257	746	266	853	258
787	266	288	251	999	601	295	231	351	677	262
601	288	314	305	242	405	188	263	275	330	257
260	254	240	153	250	172	298	280	284	271	243
253	276	263	212	267	230	275	288	309	252	251
243	260	264	277	241	322	223	277	251	291	231
278	200	241	264	259	260	256	311	302	332	235
247	273	256	243	240	288	182	281	241	225	166
257	299	530	581	549	545	510	576	546	534	509
498	227	201	265	275	219	263	232	259	314	257
225	150	167	230	280	263	281	276	110	277	271
276	23	266	239	215	162	320	308	272	160	280
285	298	258	275	204	306	309	575	245	246	256
314	187	241	244	282	250	188	310	326	246	257
296	259	291	350	293	257	321	366	279	14	291
245	252	264	235	275	191	209	289	259	215	111
272	195	237	330	307	246	256	403	240	289	61
268	305	258	211	257	230	217	275	255	281	523
231	247	338	249	303	296	677	228	221	276	195
207	373	247	139	231	656	314	333	240	166	318
227	307	310	232	307	235	260	230	251	183	279
225	268	191	264	304	322	254	175	283	249	294
279	235	327	275	542	230	239	258	320	264	246
547	460	240	259	230	260	209	263	320	231	198
171	275	312	282	249	587	424	561	248	534	302
423	486	259	321	314	536	356	279	98	248	554
224	558	497	239	255	162	238	204	268	259	255
485	400	372	387	332	388	320	361	366	235	

1735.8_1344EC63	264	283	185	282	261	260	262	594	404	237
233	242	288	312	311	403	234	342	346	312	244
348	264	383	253	309	326	306	282	344	340	329
347	337	345	373	385	246	398	303	256	252	292
210	295	361	248	179	338	273	312	285	262	348
299	334	345	335	262	307	329	634	420	622	280
617	406	265	281	601	999	251	309	370	709	270
634	369	235	380	325	429	265	303	330	326	357
341	281	342	204	376	226	333	364	327	443	271
435	321	336	267	347	297	338	228	249	461	456
305	290	297	350	335	265	199	370	331	365	320
273	195	218	324	308	307	332	257	284	401	371
311	324	256	254	267	264	238	277	219	220	239
340	229	546	583	562	542	556	592	535	534	551
572	371	340	385	391	379	367	372	385	391	393
353	241	271	332	365	361	289	297	203	324	301
361	255	324	292	303	287	381	337	382	266	300
313	368	216	209	257	262	414	602	168	253	149
278	406	304	277	413	300	232	335	376	228	293
248	212	249	308	275	396	371	322	356	216	357
184	391	336	254	294	105	213	233	320	256	156
381	109	363	212	323	270	311	336	333	347	186
308	369	306	265	338	460	255	378	306	420	742
330	289	270	317	308	272	717	255	358	314	288
144	422	357	225	345	630	241	327	351	227	438
268	373	353	316	222	268	356	300	365	272	383
192	304	209	320	252	484	307	224	328	352	447
359	345	241	345	652	347	242	348	242	357	384
559	454	234	344	305	369	158	318	399	353	335
190	350	325	372	349	665	392	548	307	592	322
490	535	432	323	365	545	498	442	307	370	569
400	589	399	320	427	187	401	300	377	386	369
529	495	446	521	437	453	361	470	426	367	

1737.0_1135ec00	299	320	199	339	343	338	359	218	299	264
265	292	693	362	231	324	341	192	318	346	336
365	207	316	582	288	322	597	388	307	361	306
314	334	230	252	275	258	315	425	337	376	272
253	667	360	246	176	273	323	254	346	788	270
312	262	264	258	327	308	257	304	264	269	281
286	288	290	288	295	251	999	283	208	262	292
250	235	519	280	247	285	194	322	222	255	234
243	259	264	338	264	197	286	307	299	279	268
282	297	301	208	281	181	286	689	556	273	271
238	236	236	249	320	244	182	264	259	265	273
226	226	189	292	303	285	244	775	264	375	237
286	304	229	210	319	552	197	278	263	295	172
256	489	236	232	247	250	249	266	290	308	244
206	252	234	248	240	233	261	228	253	263	270
251	189	245	215	267	248	200	224	114	214	235
237	171	209	253	197	205	292	229	232	203	315
325	269	68	785	309	359	324	194	215	325	173
728	303	281	257	251	301	206	313	357	258	315
299	557	317	375	298	288	420	386	261	193	267
287	319	196	174	364	222	260	491	334	275	155
226	0	294	250	354	332	317	395	255	289	29
242	93	335	262	310	290	262	303	317	294	326
220	280	374	327	266	635	329	414	245	311	260
640	309	301	163	258	275	471	265	283	172	325
211	260	333	250	651	201	248	206	240	141	272
0	233	168	303	532	255	244	152	257	331	294
236	337	733	286	244	259	390	238	744	286	248
286	23	784	303	246	435	576	543	465	264	280
220	222	390	266	280	245	152	232	241	261	323
241	255	252	329	324	286	345	246	94	280	274
243	238	111	238	234	185	250	110	297	292	240
248	236	271	279	272	300	234	289	273	241	

1745.0_1288EC30	377	281	194	261	295	328	256	203	576	141
267	484	316	349	343	350	239	320	285	326	343
491	277	646	319	253	380	348	319	595	360	574
605	594	366	403	544	242	487	371	391	308	282
256	305	453	258	206	326	275	233	317	271	414
320	515	515	511	295	343	504	235	475	240	931
250	504	948	948	231	309	283	999	310	299	275
269	350	266	323	365	337	197	286	361	449	457
465	457	461	225	456	188	508	474	495	464	458
458	492	487	251	494	201	485	224	228	489	476
330	461	466	456	310	443	227	479	311	472	388
402	256	342	449	433	336	274	232	275	396	370
337	357	209	388	316	266	229	347	252	269	190
290	269	305	338	311	321	305	353	310	407	313
308	366	334	534	536	272	503	387	495	508	504
273	270	455	447	522	520	276	330	190	269	335
316	330	263	319	276	287	314	363	394	285	279
359	279	189	224	309	256	581	229	143	487	130
269	345	399	243	378	316	273	587	509	284	341
387	217	480	549	275	340	302	333	359	106	441
286	598	238	192	425	11	236	194	449	319	154
368	0	377	237	313	228	329	277	550	553	23
257	109	353	439	261	472	250	312	591	498	434
291	285	252	255	365	231	368	185	367	296	407
195	442	440	304	415	259	218	381	181	208	545
257	497	496	444	209	201	478	379	441	188	450
387	465	149	472	213	334	482	162	491	314	488
453	464	212	426	305	377	232	460	257	413	382
386	201	301	426	461	452	311	378	433	378	412
219	441	444	403	462	357	260	282	385	289	543
305	291	375	417	397	344	455	448	216	384	326
413	373	178	453	435	75	474	184	526	525	403
242	366	315	348	343	361	253	370	308	307	

1759.0_1344EC20	289	293	278	247	253	273	290	326	447	188
237	259	336	356	504	438	260	347	630	336	312
305	235	309	252	277	424	302	251	432	289	463
420	461	413	450	363	301	405	284	295	277	341
295	229	417	279	230	459	274	210	236	225	362
258	303	307	306	260	309	308	369	325	371	295
336	386	320	298	351	370	208	310	999	362	346
387	347	233	514	345	513	176	322	354	372	336
329	367	341	308	383	205	380	333	376	332	358
333	380	369	319	377	266	374	143	263	376	375
258	359	359	359	284	272	207	449	260	448	382
268	186	177	370	333	311	206	181	288	312	246
276	257	240	223	247	247	344	251	182	191	274
259	208	319	323	327	320	307	347	333	412	318
316	321	345	331	328	293	332	299	327	313	321
295	369	263	318	332	322	217	251	217	259	256
238	289	251	278	358	170	404	287	299	378	266
398	464	169	165	254	290	463	316	166	319	141
332	455	361	278	465	350	304	419	304	285	261
297	190	272	356	218	568	322	278	479	214	440
183	401	250	286	353	114	285	251	348	302	167
441	0	402	265	251	235	291	267	398	377	156
270	164	349	451	317	402	264	317	407	368	395
279	380	262	357	360	213	369	176	309	356	404
115	392	419	250	267	368	164	502	248	222	410
305	341	356	337	187	238	360	239	360	188	337
0	379	184	356	256	494	367	206	396	294	358
319	377	255	300	401	350	248	346	244	326	290
298	193	280	416	389	443	146	378	404	335	315
153	335	375	366	307	391	274	294	265	340	376
299	338	370	370	357	336	453	329	263	399	396
312	303	134	371	333	150	308	279	335	361	247
371	328	383	428	389	412	355	426	353	336	

1770.0_1344EC63	245	276	229	304	296	214	255	635	455	233
281	284	272	282	322	424	251	252	348	282	251
351	255	381	226	273	364	309	302	368	358	337
345	342	341	350	408	252	387	265	283	248	384
265	262	351	251	190	358	325	211	287	257	313
298	334	361	348	253	280	347	707	399	674	297
678	407	286	300	677	709	262	299	362	999	271
721	328	224	344	282	457	204	370	325	332	336
340	374	333	207	322	152	364	385	352	363	349
363	335	333	254	354	276	345	193	205	379	379
290	329	333	379	304	308	180	344	302	347	301
288	234	262	339	333	304	264	288	333	320	344
276	254	240	258	248	149	208	277	267	283	200
273	152	604	670	628	608	627	654	607	608	654
582	339	308	333	351	334	314	319	352	358	355
318	189	243	328	343	340	286	296	197	298	285
376	315	297	299	238	292	316	406	311	240	312
319	349	234	196	219	255	453	640	154	294	103
258	424	317	330	255	304	233	339	363	203	248
269	136	219	309	305	364	265	264	391	152	330
201	377	201	257	284	136	283	221	343	274	175
321	241	332	271	231	200	305	309	368	378	43
237	320	262	283	197	395	165	290	293	399	573
203	352	373	300	236	189	977	112	383	231	267
140	374	434	243	292	778	174	366	216	179	404
241	371	361	294	165	276	366	248	333	201	349
177	292	208	345	218	388	351	170	365	339	378
360	376	186	310	524	297	143	281	228	344	379
548	521	189	324	329	371	141	371	368	303	268
215	322	310	352	361	631	455	608	449	641	334
574	554	335	360	368	656	452	376	181	335	628
318	617	508	302	353	94	312	149	328	306	323
478	494	347	384	313	367	347	355	315	319	

298

1782.6_1185EK08	312	310	208	436	368	272	344	222	317	317
301	340	272	411	354	319	354	380	311	360	396
398	270	340	355	278	323	315	319	287	419	287
300	288	327	289	284	195	344	402	307	352	351
621	328	347	291	228	430	419	245	298	348	277
314	281	293	295	318	356	291	281	283	241	283
308	281	269	288	262	270	292	275	346	271	999
219	250	343	330	241	301	180	358	282	284	258
267	278	269	371	302	205	285	298	301	306	265
308	299	271	247	284	225	272	223	525	325	329
268	263	261	271	322	242	314	271	261	271	276
228	310	159	265	257	218	217	240	240	336	245
281	309	298	245	426	334	246	365	325	298	251
245	409	247	280	273	257	235	287	255	316	267
262	262	295	305	289	295	312	271	294	287	310
291	231	277	278	325	293	223	238	185	200	244
257	249	217	208	272	198	338	287	265	253	408
371	394	194	238	314	344	349	216	290	307	202
271	309	322	244	443	356	302	313	381	216	391
336	330	295	374	356	281	438	370	303	487	284
352	333	256	402	324	152	624	395	305	293	175
272	0	283	261	372	427	336	348	330	302	173
349	137	376	272	353	350	532	369	313	304	302
219	315	265	356	309	337	307	256	286	974	202
209	357	292	203	246	268	279	284	283	320	471
186	260	378	262	397	191	281	181	261	154	340
4	274	170	252	519	312	256	220	271	318	368
250	277	322	282	220	325	274	296	275	304	267
314	144	301	346	303	311	213	317	354	339	306
313	287	327	323	296	316	224	289	264	257	314
296	218	302	395	420	295	416	339	185	300	320
285	284	152	264	306	209	268	135	306	298	271
255	237	355	408	373	365	265	352	310	260	

299

1813.4_1344EC13	294	248	237	286	296	227	317	571	380	234
	249	283	282	313	327	365	288	307	398	320
	303	309	330	243	268	357	298	281	361	267
	329	351	319	391	446	257	391	276	288	265
	250	252	304	277	194	340	257	225	285	231
	253	349	361	359	224	247	359	613	380	650
	604	372	276	274	601	634	250	269	387	721
	999	308	237	364	257	414	201	331	331	328
	388	323	373	201	374	182	317	384	306	404
	405	303	292	243	308	280	291	209	238	369
	259	339	344	377	255	270	218	321	259	325
	288	217	198	327	303	287	266	270	299	338
	265	247	267	252	228	157	204	258	236	226
	281	161	754	735	756	742	758	766	705	665
	665	277	268	315	331	315	302	274	338	337
	267	203	164	308	313	300	314	297	152	303
	321	193	323	282	231	273	289	382	307	241
	334	401	198	201	226	317	385	576	98	307
	281	295	325	264	327	358	215	370	320	230
	316	177	271	308	227	373	241	307	356	197
	182	443	174	263	245	126	279	222	323	267
	357	204	283	207	217	174	264	352	330	368
	200	346	241	324	231	390	130	333	346	382
	235	307	371	282	304	191	738	97	419	205
	133	354	322	320	286	906	202	387	205	127
	216	369	308	224	174	217	393	284	358	209
	174	284	196	309	215	353	353	175	364	297
	324	351	198	286	544	251	179	208	243	274
	589	580	203	337	316	297	139	293	313	258
	176	269	310	336	330	650	540	752	427	740
	676	606	385	298	339	746	375	350	279	313
	311	692	647	259	315	134	305	169	314	300
	499	571	335	359	311	400	290	334	308	230

1813.5_1313EC199	308	323	218	272	324	260	319	285	507	
243	270	336	319	312	379	379	278	276	413	390
652	307	265	331	238	281	450	345	232	455	319
429	455	459	339	424	544	283	504	287	378	298
267	221	276	421	328	270	332	315	221	278	292
391	325	374	396	395	290	322	389	283	422	290
342	268	485	346	346	288	369	235	350	347	328
250	308	999	218	342	280	377	216	315	499	438
407	419	434	414	369	418	184	429	718	438	463
425	467	432	448	285	449	245	445	191	230	536
538	243	412	413	420	280	343	212	403	274	404
360	323	194	177	362	410	363	218	223	321	314
387	272	275	245	259	252	151	272	268	291	256
253	256	187	340	355	338	340	329	344	324	404
339	354	349	288	518	546	340	498	394	545	506
507	312	284	207	482	510	513	263	320	219	359
338	309	397	328	356	296	187	351	276	385	295
286	403	341	165	190	239	319	508	294	193	327
91	296	352	439	301	352	374	734	293	287	281
274	290	173	275	326	196	424	334	266	387	202
401	168	553	193	263	364	0	217	199	402	316
254	297	110	336	261	330	271	302	218	680	412
181	276	207	334	384	196	414	242	252	388	472
445	298	331	335	293	298	208	344	111	327	270
334	146	427	381	305	646	356	172	307	261	172
459	287	694	366	246	197	325	409	512	353	212
291	541	349	152	400	205	405	446	232	455	253
451	697	477	221	637	394	278	214	261	239	641
424	280	252	279	421	380	457	244	397	369	292
224	164	257	386	432	643	403	275	344	317	320
345	531	314	326	379	394	345	415	392	205	339
377	397	410	222	554	430	157	538	247	492	522
650	288	357	341	347	319	316	348	373	316	250

301

1820.5_1185EK04	341	376	228	405	404	338	389	161	274	303
601	358	482	519	331	340	363	263	296	364	313
371	251	281	483	315	295	513	376	339	395	308
349	317	275	311	253	221	333	441	349	393	322
287	608	350	251	212	313	356	255	323	566	302
326	258	292	284	375	370	283	305	245	280	288
271	245	290	271	314	235	519	266	233	224	343
237	218	999	240	253	275	203	286	297	282	255
260	270	274	339	275	195	273	257	273	256	260
256	262	241	234	235	271	238	462	538	255	248
217	228	227	230	305	273	242	292	270	290	248
245	261	174	249	246	222	262	493	259	408	217
284	318	276	191	332	601	223	323	280	319	206
279	585	253	250	243	265	218	258	273	306	283
224	220	243	250	244	231	257	223	249	261	260
252	222	214	220	272	259	201	195	145	178	230
97	162	163	178	249	164	291	178	238	196	374
385	323	91	530	302	389	318	202	222	369	635
527	253	319	253	310	334	172	315	381	294	316
299	501	372	401	335	307	535	599	302	101	316
303	289	293	254	380	249	252	406	361	300	210
245	0	243	479	658	357	322	478	221	301	116
324	75	393	297	377	301	275	389	270	258	310
251	229	298	336	331	697	267	337	229	349	223
393	296	316	104	217	236	903	216	284	315	345
223	185	290	219	615	155	247	219	230	197	270
1	235	134	251	514	304	223	184	238	322	336
179	253	640	263	253	283	482	270	523	243	202
270	20	522	295	221	445	395	450	427	280	288
216	258	437	276	203	218	186	199	187	205	350
232	178	246	332	321	277	340	250	17	261	251
279	232	144	262	263	211	249	161	284	290	220
261	229	306	314	301	310	219	298	277	227	

302

1821.6_1288EC03	250	268	157	292	290	244	304	273	414	241
220	285	231	320	493	374	282	482	432	329	293
350	242	344	237	257	398	263	230	352	257	362
360	376	466	433	444	210	412	288	237	254	302
256	284	400	250	176	367	325	218	268	264	360
231	343	375	380	212	273	385	358	407	297	320
348	415	352	311	305	380	280	323	514	344	330
364	342	240	999	280	793	185	424	397	427	374
386	406	373	242	420	141	480	436	470	480	389
491	469	449	237	430	188	430	217	265	474	480
269	497	490	460	217	412	211	390	258	393	447
377	235	191	472	461	364	239	217	248	370	452
287	270	254	256	250	179	218	313	210	257	273
273	199	351	402	379	388	374	421	383	461	371
402	424	384	459	473	405	451	416	462	461	457
368	250	281	474	461	483	239	298	153	313	320
313	337	303	302	248	251	309	299	410	264	275
385	345	142	225	229	304	426	234	135	289	117
223	376	347	265	542	324	311	435	346	313	259
291	165	308	318	190	395	274	276	464	153	438
184	478	181	261	235	109	263	229	350	259	153
458	0	476	226	273	291	245	299	440	404	42
249	117	297	386	316	445	241	326	399	440	457
291	409	234	288	311	211	414	141	385	345	388
146	380	459	315	413	351	212	773	195	203	460
284	518	414	296	176	243	397	314	354	187	417
366	473	75	468	225	414	482	180	493	253	431
460	464	235	438	315	264	234	327	257	460	474
331	141	298	489	483	381	171	393	371	275	253
157	316	333	370	441	413	268	381	383	401	400
397	372	419	429	387	424	406	457	272	391	392
400	402	207	404	448	159	424	248	464	446	453
266	364	381	389	360	359	284	364	319	373	

303

1821.6_2011EC49	340	329	162	279	279	289	299	247	447	185
232	314	301	354	439	461	246	245	464	318	282
364	230	394	282	219	368	314	321	472	306	438
462	472	339	437	411	200	381	267	312	322	271
251	278	451	267	230	378	296	277	254	246	476
371	335	355	347	314	258	352	265	346	244	363
254	375	380	367	242	325	247	365	345	282	241
257	280	253	280	999	389	226	306	345	387	306
315	361	337	336	342	192	401	353	399	313	357
338	398	382	209	403	225	400	225	238	371	390
516	341	340	351	338	317	208	367	632	368	353
300	273	398	390	366	323	329	225	387	285	351
509	348	228	467	300	199	211	288	240	197	195
373	226	302	308	322	331	293	339	335	397	328
324	288	241	320	287	353	279	252	344	319	358
275	239	207	285	292	309	250	402	220	438	407
410	352	424	419	213	328	371	458	272	236	296
394	508	221	207	262	299	437	235	162	336	93
259	436	427	257	363	278	274	375	399	283	228
379	183	284	347	215	448	283	253	386	253	414
152	394	187	209	308	109	278	212	363	298	261
325	160	273	226	278	244	363	273	323	344	55
274	215	273	335	308	365	186	313	362	369	374
211	354	258	278	261	258	325	163	272	275	322
150	361	313	257	280	285	162	290	270	134	323
198	330	327	213	221	263	322	231	292	251	287
174	309	202	329	231	419	351	193	363	332	339
281	390	229	283	270	245	174	238	203	290	353
299	179	270	375	302	322	116	340	337	284	225
220	241	326	353	337	305	303	282	259	332	334
231	311	246	289	269	349	424	242	275	356	243
246	303	210	267	278	161	285	213	271	265	262
245	256	321	324	336	384	359	382	348	206	

1826.9_1313EC200	312	331	237	314	297	294	327	342	451
264	307	302	303	412	459	480	304	401	467
370	393	288	409	299	333	481	355	296	394
366	405	398	458	470	485	289	496	353	342
368	305	357	431	293	203	440	332	324	321
423	286	346	394	395	294	362	390	402	450
318	387	458	346	324	405	429	285	337	513
301	414	377	275	793	389	999	301	347	429
382	396	423	416	320	424	234	418	481	411
435	499	411	381	343	416	285	390	249	316
507	415	428	432	456	275	401	243	453	364
462	392	277	214	461	470	401	405	256	330
453	399	377	340	252	311	273	307	312	253
299	407	281	360	389	375	372	342	402	368
414	434	429	392	443	446	425	441	418	437
426	398	302	292	457	451	472	281	375	234
385	382	387	358	341	332	308	446	356	445
326	449	424	202	239	267	327	462	323	198
173	279	452	416	347	468	330	367	468	413
299	317	265	304	351	240	490	384	347	474
482	247	547	233	305	349	144	317	276	442
188	489	118	548	312	358	327	311	388	482
194	321	181	390	475	381	536	278	400	379
485	438	474	300	378	359	292	455	272	411
417	156	434	493	377	437	413	266	955	382
502	327	497	408	332	251	331	421	323	403
430	266	384	222	420	316	457	438	246	461
498	475	491	294	464	427	388	315	377	303
491	419	314	331	454	424	419	211	435	390
362	240	369	391	448	465	453	348	384	372
413	427	426	441	470	437	396	530	474	336
507	425	393	244	412	460	214	484	305	459
417	384	428	548	552	512	530	398	497	486

1843.5_2011EC47	210	294	187	195	196	219	205	184	225	129
195	210	194	216	174	208	191	184	200	275	221
270	199	298	208	173	192	191	220	209	240	193
215	185	195	232	248	220	240	226	187	260	179
197	184	215	248	222	285	204	609	237	189	197
364	216	179	181	205	182	183	278	197	197	166
234	216	215	174	188	265	194	197	176	204	180
201	216	203	185	226	301	999	152	248	253	190
187	190	189	156	189	313	184	208	184	213	203
215	179	171	211	182	352	191	209	199	225	253
283	188	189	205	239	170	207	208	268	207	175
160	198	222	173	177	160	255	170	325	248	234
261	337	297	238	217	224	198	200	254	219	182
292	203	206	292	229	241	240	281	290	349	259
230	167	185	168	169	338	174	188	227	244	225
316	187	235	178	183	188	243	232	50	243	257
197	93	238	171	181	118	312	248	202	169	190
251	268	244	135	214	205	215	166	120	224	102
159	69	259	177	215	170	171	211	283	139	215
167	214	202	205	230	199	221	246	153	127	184
176	240	169	127	210	205	184	169	199	231	215
199	264	216	160	248	184	368	192	189	202	37
235	96	201	167	219	205	196	205	180	209	272
203	120	209	208	181	217	173	148	191	209	115
155	222	136	163	230	174	193	198	361	155	231
204	175	210	231	208	226	188	162	189	240	215
139	140	281	178	204	209	187	208	197	228	214
185	190	214	204	196	301	199	242	191	185	189
180	6	101	240	174	161	147	144	181	323	269
184	243	183	238	204	165	258	130	194	202	146
147	193	187	218	205	254	291	198	188	188	173
151	220	86	161	214	161	162	194	181	161	184
199	140	314	318	269	338	288	303	285	229	

306

1853.9_1164EK02	287	273	166	175	196	288	335	275	410	233
211	235	344	379	395	446	292	477	341	318	247
298	289	337	339	233	383	354	259	355	307	365
350	361	339	364	384	216	382	367	259	276	222
266	357	386	215	198	351	326	197	202	354	347
262	351	353	342	259	318	337	282	412	293	279
269	419	334	286	263	303	322	286	322	370	358
331	315	286	424	306	347	152	999	342	399	403
428	408	423	215	412	220	439	444	441	448	385
433	426	394	216	398	140	409	258	368	411	417
197	418	414	397	226	301	219	386	233	385	394
306	185	217	413	374	340	212	267	194	396	350
230	291	218	235	257	307	191	239	198	197	272
203	321	323	402	307	317	308	323	342	370	351
343	379	296	411	395	339	362	341	360	350	382
325	210	287	340	378	385	191	267	292	221	270
280	207	211	264	194	280	312	314	353	216	236
396	355	157	332	289	335	411	330	265	264	229
333	415	375	255	473	290	193	368	351	331	379
319	254	277	369	227	304	277	322	364	17	361
161	448	132	260	309	32	261	323	384	246	125
404	0	408	226	284	333	289	341	340	390	160
277	121	338	374	201	419	431	301	389	442	453
337	331	288	315	390	302	400	278	322	396	386
243	396	343	271	306	317	266	282	182	349	515
213	355	492	266	303	185	439	265	429	151	489
0	397	200	445	333	395	416	187	427	280	426
332	364	287	364	267	273	245	327	264	372	328
355	308	344	469	442	453	306	404	450	280	327
117	313	394	343	343	408	217	326	328	339	389
369	337	393	457	445	418	433	410	264	375	381
355	406	249	325	402	183	369	133	374	397	344
258	356	313	354	286	366	220	345	318	325	

307

1854.9_1164EK03	318	303	186	289	278	290	330	257	478	250
257	258	304	351	465	450	288	379	427	347	370
352	274	356	251	454	389	299	278	410	271	401
405	395	369	466	519	247	497	290	276	249	293
298	319	422	276	273	289	268	275	256	255	389
295	435	458	463	251	301	452	282	469	285	359
263	482	378	366	275	330	222	361	354	325	282
331	499	297	397	345	429	248	342	999	417	425
433	403	431	316	448	186	470	532	461	501	426
502	452	444	304	451	228	448	173	257	515	500
270	451	455	467	276	380	165	382	282	382	435
397	212	173	478	465	428	273	221	295	318	488
303	293	274	226	278	197	310	320	242	234	295
298	196	304	375	297	319	302	344	313	483	346
444	381	331	479	486	328	468	447	481	503	497
350	336	294	588	456	460	253	666	489	379	671
324	400	410	564	329	256	374	265	462	330	295
401	353	139	197	272	330	476	243	225	296	153
286	423	395	414	439	364	402	376	350	346	281
317	207	298	337	186	452	356	294	448	213	465
168	514	247	288	298	30	304	225	377	285	229
429	6	423	263	319	226	303	292	524	445	164
270	174	320	444	290	479	220	371	455	497	463
320	375	319	334	325	254	329	298	456	314	436
236	401	489	409	521	308	230	383	272	233	484
302	594	426	288	219	290	445	379	428	204	408
325	381	201	425	245	462	456	271	466	298	457
569	512	241	461	370	292	266	361	279	472	538
353	222	331	452	450	563	230	469	528	285	256
184	338	385	370	474	418	297	340	392	337	413
375	354	462	450	436	335	459	481	264	441	440
479	404	193	463	507	203	479	244	488	480	493
351	401	370	399	375	378	382	403	333	369	

308

1862.2_2011EC39	277	297	201	304	303	296	315	287	611	246
277	305	312	377	431	429	309	344	381	351	338
445	247	477	310	271	424	333	311	497	402	492
505	492	443	466	738	248	629	416	333	293	306
313	352	510	287	236	388	335	265	310	292	463
320	643	642	637	300	291	633	335	648	301	428
318	680	447	437	330	326	255	449	372	332	284
328	438	282	427	387	438	253	399	417	999	681
693	976	687	364	675	206	544	550	545	661	971
662	524	530	204	547	241	537	223	288	619	620
332	550	561	649	328	372	244	439	326	444	466
394	304	278	575	541	382	334	254	331	387	517
342	360	240	291	296	321	191	338	278	300	205
334	267	342	438	356	336	349	388	364	451	346
420	461	431	550	546	413	500	441	645	529	627
431	207	296	537	452	472	202	389	301	415	402
446	335	423	415	197	338	404	446	409	221	332
370	434	167	238	267	315	624	297	244	314	184
294	397	464	319	391	386	310	413	468	261	303
253	237	266	334	328	353	282	308	448	145	474
198	702	175	292	347	211	291	278	489	302	215
431	118	477	339	334	289	363	327	673	647	227
325	200	362	445	318	623	268	412	552	700	457
384	325	293	307	399	307	359	299	572	307	578
187	531	528	442	478	295	271	356	347	234	592
285	584	535	322	251	335	736	340	716	260	544
334	497	197	530	290	361	617	258	633	375	616
543	564	235	556	308	334	316	322	287	527	526
408	307	326	538	551	586	372	445	573	384	354
261	332	607	569	524	500	275	340	510	365	589
373	360	524	555	543	431	498	511	379	515	434
471	379	221	442	493	147	477	253	467	489	505
332	396	367	425	359	422	320	454	403	363	

309

1865.3_1135EC00	276	272	118	296	296	302	253	252	635	247
268	300	280	364	370	406	284	306	398	313	320
424	250	477	298	262	387	310	323	507	420	482
495	484	396	478	832	181	730	360	265	255	264
263	320	537	298	204	275	251	243	284	230	477
316	887	898	902	244	319	888	312	834	264	424
302	797	434	430	257	357	234	457	336	336	258
384	407	255	374	306	382	190	403	425	681	999
975	709	942	306	908	159	590	593	610	772	680
771	572	587	129	613	112	612	203	229	716	719
291	667	682	804	344	438	182	419	301	427	453
451	197	275	617	589	392	248	218	259	378	573
319	321	204	300	307	235	118	338	235	235	128
285	233	385	465	397	372	412	437	407	425	370
465	579	405	580	583	384	558	519	721	576	717
415	143	283	603	529	543	167	378	255	439	383
381	369	404	449	152	300	324	430	491	179	327
396	337	135	195	274	253	646	264	232	313	173
303	371	510	218	342	345	305	428	450	247	286
230	221	241	342	324	362	266	286	381	185	484
139	782	225	223	294	60	241	247	499	293	194
377	0	401	226	292	217	332	290	636	915	33
231	172	364	436	271	724	243	442	565	806	507
347	348	202	254	460	236	374	175	646	277	705
172	560	552	457	494	278	247	385	221	166	614
227	610	581	301	200	319	966	353	921	147	586
392	528	131	573	222	383	688	183	703	379	705
561	621	225	527	353	249	258	298	223	495	545
457	338	316	556	614	626	428	458	634	270	284
247	294	597	476	552	547	265	368	637	436	597
404	360	583	579	527	458	438	608	338	524	409
521	453	246	380	571	139	475	229	541	539	512
229	420	279	338	296	366	239	371	295	301	

310

1866.7_1185EK18	287	299	180	306	306	311	259	267	628	245
263	310	285	383	376	453	290	330	384	329	328
431	252	488	296	265	387	320	334	518	432	495
506	498	389	512	825	216	727	387	275	259	278
292	315	546	310	219	301	268	248	296	234	480
343	882	894	897	254	321	883	321	819	277	427
319	791	441	435	260	341	243	465	329	340	267
388	419	260	386	315	396	187	428	433	693	975
999	724	941	303	933	160	594	593	615	785	690
771	578	591	160	618	180	621	195	241	693	694
285	653	667	788	357	443	171	426	303	432	478
454	202	281	640	608	426	237	199	284	379	572
322	345	213	299	289	249	151	322	233	241	175
269	210	388	485	402	377	414	445	406	434	377
473	580	406	577	579	393	557	517	701	572	711
427	172	305	591	529	537	218	377	256	433	383
372	374	400	439	197	317	321	430	488	201	331
404	361	176	181	280	259	643	277	236	324	158
299	424	520	243	342	349	297	378	453	259	283
238	181	261	356	332	366	280	310	388	206	518
142	781	193	260	298	26	256	281	491	313	200
360	0	414	228	298	240	339	311	641	911	39
276	175	371	443	277	717	246	446	595	799	525
333	349	229	254	449	220	380	124	640	273	701
158	565	578	465	483	285	243	391	216	141	625
231	605	567	318	212	379	960	349	930	186	586
375	521	136	574	230	396	685	200	697	392	704
556	635	197	526	314	296	242	334	230	495	550
458	342	314	555	621	627	431	479	646	322	336
237	328	637	469	545	569	288	372	631	443	603
404	344	590	564	532	477	461	609	333	530	414
519	446	243	381	565	88	476	208	542	543	524
229	441	293	357	320	361	255	375	279	327	

1869.2_1344EC16	300	291	140	311	311	295	326	240	655	208
268	310	302	381	434	489	319	323	404	375	337
433	259	491	309	262	420	321	318	538	410	527
524	515	381	464	759	157	655	421	306	275	291
323	329	490	291	219	390	289	226	308	255	447
328	692	693	691	289	278	687	289	684	265	425
298	723	452	434	254	281	259	457	367	374	278
323	434	270	406	361	423	190	408	403	976	709
724	999	712	374	726	159	575	553	572	675	975
675	553	583	115	598	125	593	200	252	632	632
314	545	555	658	321	363	228	443	269	444	420
396	269	251	545	500	353	227	219	280	372	525
301	324	246	277	267	298	107	304	265	284	163
249	262	379	486	387	377	408	454	417	440	312
433	495	414	540	549	394	528	477	672	553	666
381	112	291	526	484	497	158	379	271	411	397
407	335	398	437	119	324	332	415	438	134	335
387	440	148	212	268	326	659	254	190	334	151
294	451	483	256	352	397	294	403	453	249	307
280	191	240	350	314	386	266	311	415	138	478
204	726	128	292	326	27	289	296	476	307	193
400	0	444	306	306	240	338	291	683	697	246
269	145	340	425	277	677	236	404	596	726	489
361	348	257	295	379	273	400	159	615	293	634
158	549	527	492	466	283	217	429	229	199	578
271	582	510	303	226	318	762	322	740	150	512
318	483	152	507	243	437	631	177	654	356	627
536	576	212	505	284	257	305	335	263	449	526
420	263	313	516	541	567	388	443	586	286	265
230	331	610	528	515	515	268	339	543	395	619
401	419	551	518	503	467	485	564	306	507	369
506	346	237	463	513	101	482	226	500	516	497
263	411	290	346	310	389	247	388	313	307	

1870.1_1135EC00	288	279	134	332	325	296	290	229	625	235
275	310	311	378	401	430	303	312	420	340	326
437	256	473	311	248	397	340	324	510	452	479
496	485	405	502	822	173	719	373	310	266	300
288	326	551	325	192	342	283	218	346	253	492
329	885	911	909	296	336	900	320	803	253	432
309	812	443	439	240	342	264	461	341	333	269
373	414	274	373	337	416	189	423	431	687	942
941	712	999	280	964	147	601	595	619	781	687
764	585	604	149	637	125	620	218	253	682	686
289	634	647	807	353	467	181	448	324	455	460
413	204	293	608	582	404	269	213	287	390	575
340	334	246	315	312	249	133	357	244	254	133
289	234	415	494	434	406	417	452	419	450	398
445	554	425	547	557	407	555	500	737	569	733
442	147	262	603	519	530	181	393	312	503	399
454	440	473	525	157	362	319	506	469	161	361
411	357	105	221	290	290	639	248	204	334	149
294	423	503	227	354	366	319	406	455	239	293
265	240	237	348	368	382	268	318	364	156	505
205	799	180	244	278	62	258	251	500	332	195
397	0	395	229	300	214	352	321	625	906	118
242	168	381	396	290	703	220	433	576	818	521
347	354	217	249	439	247	365	171	608	266	661
184	532	591	466	503	293	229	408	236	174	626
216	626	558	285	212	295	945	344	954	164	595
392	496	149	533	225	372	695	198	717	380	683
587	620	246	541	321	255	284	285	226	511	564
447	256	325	553	572	633	405	487	655	265	278
237	281	627	456	550	584	273	389	613	448	613
416	343	586	588	545	472	436	607	320	536	408
497	452	243	394	550	140	482	220	532	533	553
260	453	266	342	298	381	219	358	298	308	

313

1871.6_1164EK04	312	246	3	267	273	260	292	148	296	229
219	285	387	302	349	412	340	203	363	709	439
331	120	292	362	265	328	411	346	316	350	358
341	338	324	364	311	2	292	303	466	353	290
240	350	367	307	142	364	329	174	290	329	336
269	223	249	239	329	563	226	202	286	170	291
217	309	211	293	153	204	338	225	308	207	371
201	369	339	242	336	320	156	215	316	364	306
303	374	280	999	284	103	294	279	297	229	363
234	277	255	3	257	156	261	177	343	252	255
195	278	278	299	287	322	281	306	149	308	269
232	317	180	237	276	246	137	247	244	380	218
158	244	228	239	392	319	5	395	360	372	124
172	253	206	241	207	209	203	242	283	291	185
265	247	286	254	240	220	275	234	259	256	282
248	3	131	215	251	233	153	319	131	263	291
275	220	293	269	7	129	226	262	197	3	262
462	407	1	255	308	292	278	92	243	327	44
321	380	339	296	243	655	275	224	313	232	220
342	62	274	330	308	352	288	319	362	207	347
359	305	188	515	469	0	229	236	332	260	146
276	0	246	234	336	287	302	378	362	284	151
103	43	564	286	276	228	272	322	313	319	301
229	317	235	242	244	303	277	78	277	369	265
127	304	262	308	276	242	264	351	107	106	308
179	336	235	195	269	281	302	178	280	1	224
29	215	1	312	311	342	310	247	318	366	325
309	332	301	343	218	105	259	101	323	365	235
252	153	334	294	287	336	121	308	323	146	149
311	102	348	325	332	257	159	231	219	214	294
286	273	226	321	288	275	320	258	129	279	200
258	200	5	340	242	208	288	5	264	290	296
176	238	175	174	177	222	214	213	176	189	

314

1875.4_1185EK18	294	325	146	303	289	300	278	269	625	256
272	313	302	395	380	445	292	310	407	348	348
425	242	490	332	259	426	345	349	539	454	515
541	535	410	490	805	180	712	407	300	299	291
306	333	544	302	220	354	284	237	319	262	477
328	841	872	869	280	327	858	336	822	277	418
329	789	429	428	250	376	264	456	383	322	302
374	418	275	420	342	424	189	412	448	675	908
933	726	964	284	999	175	603	608	620	774	698
752	586	601	126	628	102	627	213	256	696	699
294	615	627	784	344	453	185	473	297	480	490
457	246	235	645	612	417	223	181	273	388	573
311	356	237	262	313	257	118	355	235	243	130
258	245	403	498	418	395	420	439	401	448	393
482	553	428	576	584	416	571	511	731	577	744
422	122	258	583	530	536	197	378	251	425	378
347	360	404	448	132	307	304	415	469	145	333
415	361	172	209	274	278	642	269	245	356	156
309	432	505	237	364	368	302	420	457	247	293
279	198	245	372	345	374	291	331	422	176	498
182	786	237	282	319	26	271	286	493	304	204
431	0	402	246	307	254	320	328	639	889	144
274	198	372	450	306	738	227	435	577	797	541
347	375	245	273	440	237	379	144	694	310	677
171	552	571	447	486	278	245	425	222	171	636
233	615	554	289	234	295	910	348	952	137	591
386	490	138	528	241	422	690	183	704	375	691
564	673	240	527	331	249	238	284	242	498	559
450	337	312	562	576	633	427	484	677	295	302
219	278	680	451	551	597	273	381	613	451	622
423	376	597	573	521	485	463	611	322	536	421
519	465	268	383	553	92	477	261	543	552	527
257	461	284	344	294	363	247	373	272	310	

315

1879.6_1344EC04	227	237	284	189	186	218	203	166	152	163
207	209	227	213	250	209	213	237	145	208	188
215	179	184	210	197	154	242	282	167	250	137
168	155	167	225	154	318	201	210	187	255	227
193	213	129	225	131	234	220	261	139	238	218
231	154	161	144	268	212	149	219	112	175	171
175	142	193	178	172	226	197	188	205	152	205
182	184	195	141	192	234	313	220	186	206	159
160	159	147	103	175	999	114	154	115	163	148
176	137	134	294	144	351	141	243	197	160	176
230	111	111	113	261	140	166	140	230	127	125
185	181	175	139	129	159	255	153	275	240	191
281	226	328	208	189	261	299	201	223	47	182
288	213	194	204	216	212	203	242	232	265	236
219	179	170	158	161	364	147	208	178	186	187
298	288	215	144	138	137	233	143	155	135	238
186	89	218	130	297	154	268	225	185	287	217
217	179	172	175	223	203	131	190	210	233	273
209	138	141	253	159	165	95	127	206	161	257
126	175	225	164	240	236	275	238	178	192	182
66	166	160	181	176	233	195	221	143	221	109
213	170	156	196	214	188	276	161	139	156	24
182	103	220	143	130	123	221	170	127	107	219
215	145	190	287	129	231	110	55	143	240	106
124	163	115	164	178	71	215	107	376	246	188
136	169	167	202	248	153	124	137	131	676	190
129	169	223	146	257	140	122	197	117	239	150
164	146	236	157	85	294	269	222	208	144	209
155	196	122	181	103	124	94	128	146	333	303
144	222	144	199	141	163	258	183	208	135	141
129	147	198	141	165	198	245	156	141	159	146
183	179	50	123	233	215	113	259	149	129	150
247	92	279	306	245	231	289	253	254	209	

316

1879.8_1185EK17	309	322	194	335	322	305	355	251	653	292
285	345	320	371	416	456	335	339	400	367	379
434	259	476	279	273	442	330	306	640	376	627
654	662	410	477	678	254	617	356	377	324	342
333	322	549	338	196	347	339	206	276	318	455
324	609	616	619	298	303	608	303	724	299	483
309	756	539	483	298	333	286	508	380	364	285
317	429	273	480	401	418	184	439	470	544	590
594	575	601	294	603	114	999	584	970	641	555
660	982	969	242	905	156	940	218	292	643	642
313	812	801	758	323	434	240	529	268	511	579
413	345	244	665	634	340	272	203	311	396	529
325	369	269	284	303	248	209	309	292	260	233
277	269	446	493	461	441	463	465	441	452	382
439	519	342	680	668	366	648	466	629	636	623
359	248	337	597	601	599	207	360	190	342	369
341	309	335	371	258	187	330	396	468	277	350
417	476	171	208	305	355	671	233	273	360	129
297	447	476	231	393	349	342	406	416	257	281
389	202	423	483	264	418	306	317	397	200	468
237	709	150	255	324	23	323	247	532	286	223
396	0	408	230	342	261	317	337	611	619	28
314	124	355	396	304	658	257	390	542	759	476
349	378	268	259	421	206	378	106	530	296	506
184	510	605	440	527	283	198	409	268	204	591
305	584	679	338	218	316	600	349	575	109	690
346	921	161	915	254	428	839	245	838	340	630
563	654	244	702	311	306	264	358	245	697	556
459	214	301	778	847	672	342	491	560	327	350
217	356	521	516	559	501	320	440	491	485	617
421	397	488	520	482	475	474	546	257	458	411
470	448	243	511	526	148	576	180	604	591	581
269	417	314	388	281	372	244	395	316	350	

1879.9_1344EC77	315	353	157	326	341	332	305	273	647	232
295	382	331	326	389	414	274	360	401	401	561
405	260	450	279	245	476	377	315	503	427	471
516	531	432	486	714	193	643	386	403	303	344
276	307	546	353	218	417	374	257	297	346	446
351	522	521	518	297	387	517	360	631	307	455
357	664	473	462	280	364	307	474	333	385	298
384	718	257	436	353	481	208	444	532	550	593
593	553	595	279	608	154	584	999	601	646	537
648	589	621	211	615	177	606	245	315	669	669
328	561	567	592	314	464	271	485	336	490	500
447	260	279	541	546	424	286	258	354	387	507
327	362	241	319	275	170	223	268	338	303	255
305	209	417	472	433	409	432	470	425	461	432
449	500	417	663	691	407	625	513	676	632	658
441	235	280	605	636	643	239	406	218	384	398
369	375	357	400	243	228	352	398	511	253	342
432	426	153	177	306	305	658	244	144	400	150
294	405	462	246	394	330	558	423	381	317	269
295	140	297	401	300	414	305	369	428	274	494
268	738	105	265	340	13	277	264	504	323	283
410	0	409	287	398	301	345	307	695	581	109
230	197	402	395	318	609	197	360	492	690	563
355	305	290	265	425	230	421	124	510	303	515
140	502	600	357	716	359	234	394	203	196	605
295	803	574	303	194	229	605	746	546	144	491
469	515	187	545	253	479	621	187	634	356	653
800	611	233	756	393	280	198	350	283	753	575
399	134	253	558	556	638	341	478	586	317	251
236	350	560	499	752	568	252	409	486	427	503
571	378	522	487	490	510	502	559	259	452	426
518	488	163	533	560	136	686	184	651	663	747
347	456	335	345	331	389	243	395	320	291	

1883.7_1185EK19	318	328	188	347	333	301	340	229	656	286
293	355	325	376	409	470	336	340	406	373	378
449	254	490	290	276	429	348	326	638	382	628
652	663	405	475	707	245	640	354	362	315	342
342	315	525	325	197	346	345	202	283	311	461
345	650	654	653	292	289	643	297	743	288	468
301	778	526	469	284	327	299	495	376	352	301
306	438	273	470	399	411	184	441	461	545	610
615	572	619	297	620	115	970	601	999	662	557
682	972	955	243	928	188	934	221	281	658	658
295	841	830	787	345	424	216	506	271	488	583
402	344	251	673	636	330	274	203	311	393	556
330	373	273	292	322	254	218	333	278	270	251
278	285	439	494	455	442	464	459	451	447	381
446	516	341	693	682	368	648	463	641	641	638
356	273	341	613	599	607	218	358	240	366	361
379	364	354	393	282	278	329	443	459	304	363
418	466	173	208	295	340	675	229	271	367	130
301	466	472	245	399	357	354	409	436	261	285
384	203	415	474	288	416	309	319	390	201	467
232	711	148	262	314	20	332	249	512	294	202
397	0	426	237	335	253	350	356	623	638	24
317	118	344	398	303	656	253	397	549	794	482
358	377	276	279	416	207	361	116	532	293	509
184	492	598	452	539	285	198	404	269	202	593
292	602	674	330	220	341	640	360	610	153	696
364	920	169	903	256	429	866	243	861	353	640
573	658	246	681	300	319	266	363	236	672	594
471	225	330	797	858	667	317	506	556	329	357
201	360	523	502	578	507	320	433	508	482	640
410	397	509	512	478	480	478	553	265	471	400
475	451	236	517	521	151	583	188	605	588	590
258	407	315	396	290	368	270	397	314	343	

319

1884.8_2011EC37	272	281	140	346	310	288	326	246	627	252
250	364	278	356	417	394	269	442	416	361	393
465	266	491	286	251	446	325	358	497	429	460
487	466	488	545	838	178	740	384	357	285	384
240	315	674	353	186	358	350	245	255	298	614
337	684	699	700	286	348	692	334	803	307	439
330	800	480	445	271	443	279	464	332	363	306
404	463	256	480	313	485	213	448	501	661	772
785	675	781	229	774	163	641	646	662	999	654
993	638	649	184	680	198	655	257	273	885	885
319	635	645	761	377	518	256	453	356	462	568
499	208	284	702	669	538	300	251	371	452	633
375	378	253	350	328	176	202	356	265	269	240
336	206	417	514	433	416	430	477	421	470	466
485	630	518	650	664	494	622	592	732	620	735
502	233	317	646	597	615	206	414	181	433	425
388	368	403	436	224	276	418	434	587	265	355
454	407	177	253	272	326	657	240	175	366	141
256	411	534	246	503	343	401	424	463	370	266
293	202	258	326	335	384	330	336	402	217	539
189	792	191	313	318	117	242	252	605	358	191
462	0	490	273	364	319	370	319	609	760	212
243	157	404	509	324	710	204	487	617	819	600
340	323	227	280	423	227	369	182	691	333	730
166	531	668	443	614	295	237	421	251	179	668
303	718	629	304	173	231	790	437	744	155	630
313	544	173	571	242	446	718	186	730	390	793
656	711	215	596	356	285	189	336	285	589	686
467	179	366	608	597	673	390	537	634	317	293
210	313	602	517	650	601	296	431	688	452	563
476	380	711	584	581	513	495	723	411	532	479
625	490	210	441	655	181	594	226	630	631	680
380	536	358	394	371	385	285	420	335	338	

320

1886.0_1344EC16	284	278	169	305	306	295	314	234	635	209
277	299	297	388	425	460	314	332	388	358	335
441	251	479	301	241	411	321	291	525	393	517
514	502	391	457	751	166	632	421	303	271	287
319	339	504	287	211	386	282	225	298	250	450
325	668	672	669	279	268	664	299	663	259	432
282	684	459	442	243	271	268	458	358	349	265
334	425	260	389	357	435	203	385	426	971	680
690	975	687	363	698	148	555	537	557	654	999
654	535	554	127	576	168	567	205	248	602	601
310	523	534	636	323	382	218	429	268	435	426
371	270	261	534	512	358	226	211	285	391	516
295	325	242	278	255	296	115	321	274	289	169
242	258	379	476	399	382	406	438	399	432	334
445	483	425	535	542	396	517	467	662	535	659
403	122	291	517	474	484	207	386	257	431	399
413	349	413	451	147	319	335	432	427	141	330
355	442	136	214	267	314	642	244	193	317	156
293	437	464	253	356	383	300	388	460	246	294
268	194	232	331	301	353	268	321	406	140	467
204	712	162	278	322	28	301	283	496	302	186
419	0	523	333	304	240	337	312	665	671	247
271	189	330	451	271	636	224	396	593	696	484
354	342	276	310	397	272	385	171	609	267	579
150	550	538	501	452	275	255	350	225	208	571
201	574	496	288	229	336	737	317	722	188	518
317	471	146	513	237	429	604	183	626	358	612
532	569	208	524	311	250	302	311	260	490	517
405	242	311	500	520	560	379	458	583	303	290
243	310	613	536	509	527	258	355	531	404	595
387	404	528	524	519	466	462	551	293	491	378
496	371	248	459	499	100	481	219	490	501	489
276	421	274	329	294	369	260	363	290	308	

1886.5_2011EC38	280	296	188	347	312	291	320	246	625	236
252	357	275	369	401	394	254	446	415	357	404
471	268	490	287	267	448	334	364	501	430	468
489	472	489	546	838	229	743	388	358	290	380
253	321	676	358	187	379	354	257	277	298	616
334	709	713	718	279	351	709	327	802	299	434
328	801	476	440	253	435	282	458	333	363	308
405	467	256	491	338	499	215	433	502	662	771
771	675	764	234	752	176	660	648	682	993	654
999	660	670	210	702	206	678	259	288	887	888
316	635	645	759	372	535	255	453	358	462	576
516	208	282	703	670	541	287	250	382	460	630
344	388	254	351	324	186	227	374	267	273	248
330	212	435	512	452	435	449	496	440	471	467
485	630	524	665	679	490	637	590	733	632	725
507	264	318	651	609	625	219	416	167	434	426
396	370	404	437	265	278	411	434	596	306	356
464	409	162	227	276	320	655	242	146	362	139
267	411	541	269	505	351	403	424	469	375	290
307	228	259	329	335	387	343	349	402	285	538
188	794	191	312	320	107	263	235	620	357	184
461	2	487	271	371	322	367	339	608	795	154
273	165	405	516	342	707	187	484	609	819	600
333	351	199	296	429	236	370	215	691	345	732
174	523	668	443	615	297	242	439	265	184	671
290	715	620	309	186	240	788	438	721	170	636
308	551	171	576	257	426	718	210	731	385	792
651	713	213	601	350	313	197	353	290	595	681
472	179	366	606	597	655	390	521	620	333	303
214	334	588	513	654	589	309	455	672	477	565
478	381	716	584	587	514	500	721	405	533	479
626	489	242	469	651	175	594	228	642	642	680
386	562	354	403	390	386	277	430	329	355	

322

1889.8_1185EK16	296	313	199	318	307	282	331	230	656	273
274	315	310	376	423	495	326	327	396	366	347
421	258	494	274	272	436	350	290	646	362	632
660	668	407	475	681	265	622	342	351	305	324
316	316	533	307	199	333	340	193	264	291	453
330	604	622	617	279	286	606	285	724	276	469
290	752	527	469	276	321	297	492	380	335	299
303	432	262	469	398	411	179	426	452	524	572
578	553	585	277	586	137	982	589	972	638	535
660	999	965	228	899	143	935	221	267	639	639
283	813	802	757	326	430	188	500	255	482	575
389	339	227	659	622	325	269	203	304	388	549
311	366	251	261	282	255	205	309	263	287	212
278	270	434	479	447	438	457	450	440	443	358
438	506	312	687	671	353	641	451	633	635	623
339	242	340	599	594	602	206	332	193	330	338
324	311	319	339	262	198	322	369	454	272	337
421	451	150	211	274	331	673	247	278	347	131
306	435	468	234	385	344	317	401	423	264	283
398	205	412	489	268	428	299	303	403	208	474
209	693	149	265	316	24	306	235	525	271	194
394	0	407	213	324	240	328	328	609	620	28
301	117	342	394	291	641	263	388	536	768	469
348	379	247	238	406	196	361	109	510	293	498
186	491	573	449	529	289	198	402	256	209	586
231	587	679	342	217	290	586	359	576	95	693
244	923	157	909	241	428	839	224	834	335	631
567	644	235	703	308	302	273	360	229	699	571
465	224	324	780	846	654	311	498	542	309	358
211	345	491	478	560	482	310	429	486	473	621
407	396	493	509	472	499	464	540	278	462	390
461	431	244	519	516	157	586	184	599	583	583
257	402	302	392	278	366	253	392	315	351	

323

1894.9_1185EK17	285	328	187	310	273	275	299	216	681	249
232	327	310	367	382	481	289	309	410	377	370
404	242	484	257	249	429	353	285	660	359	663
668	682	387	441	711	227	637	333	316	290	311
301	274	545	320	210	325	332	190	256	268	436
327	630	636	633	248	285	624	255	748	272	462
264	785	514	456	263	336	301	487	369	333	271
292	448	241	449	382	381	171	394	444	530	587
591	583	604	255	601	134	969	621	955	649	554
670	965	999	169	929	160	982	199	247	642	640
267	823	812	768	319	427	193	501	241	481	536
373	331	196	637	605	323	266	192	284	367	537
292	375	227	234	266	253	161	326	251	259	223
276	261	431	466	443	419	448	459	450	424	361
406	493	346	673	663	357	628	452	645	637	630
358	224	328	599	586	602	198	304	208	303	311
293	314	292	310	235	162	312	323	458	241	331
438	464	192	194	268	299	699	237	269	342	126
325	436	489	228	385	345	326	413	416	263	270
374	198	424	476	253	374	281	286	405	218	477
130	715	174	254	300	16	305	240	514	292	176
405	0	393	175	304	245	314	296	637	650	32
293	101	337	408	301	683	261	384	533	800	481
356	388	326	244	382	167	360	112	494	285	519
187	486	580	429	532	291	162	397	264	201	572
243	605	707	339	193	261	608	378	598	70	701
260	920	160	918	236	440	849	195	849	331	644
593	637	186	707	302	272	256	350	234	697	531
454	332	319	798	861	666	369	512	567	296	315
209	339	487	479	569	478	311	430	482	466	624
420	399	509	477	452	505	494	547	317	512	394
468	423	216	487	515	130	593	209	584	607	596
254	426	299	387	281	351	259	386	300	326	

1900.0_1135EC04	179	232	700	171	174	119	185	195	155	173
315	111	180	170	194	159	159	247	271	275	109
150	235	125	164	302	153	200	118	167	203	62
196	134	245	156	82	801	351	140	199	235	305
254	187	164	187	135	263	237	174	241	195	183
194	224	203	206	189	139	214	233	32	206	228
259	107	242	247	212	267	208	251	319	254	247
243	285	234	237	209	343	211	216	304	204	129
160	115	149	3	126	294	242	211	243	184	127
210	228	169	999	299	175	260	369	214	263	256
112	111	70	101	232	233	177	283	230	269	316
244	173	207	91	95	125	199	174	199	235	193
213	199	279	207	202	223	935	246	450	103	267
224	197	275	242	318	297	259	309	230	269	305
277	159	186	209	193	271	210	152	205	225	213
290	891	129	203	200	194	259	181	52	246	204
149	3	161	0	869	169	279	251	211	874	163
106	220	293	240	167	185	117	146	172	59	235
168	0	258	278	212	170	0	0	120	0	176
94	179	117	92	173	271	306	175	179	156	71
126	75	200	59	86	192	243	68	96	109	14
140	129	123	183	216	218	191	163	65	208	47
187	125	151	179	77	154	167	218	180	44	299
110	20	6	432	115	199	164	126	69	235	0
148	244	23	0	139	2	188	52	205	192	225
240	142	158	172	212	174	49	25	108	141	144
0	202	140	50	202	92	86	226	65	66	203
57	179	156	81	204	277	210	252	173	110	116
91	1	49	305	86	117	108	32	154	267	300
151	263	242	91	96	246	134	76	128	107	2
11	131	310	62	279	66	261	80	19	215	199
43	199	5	118	205	5	203	147	108	58	40
256	61	309	356	198	160	162	174	139	161	

325

1906.6_1185EK19	291	332	259	321	289	293	289	229	697	238
230	341	302	369	398	453	276	339	426	375	378
434	230	497	261	260	450	343	300	649	390	650
656	665	403	450	725	313	673	334	326	290	299
245	302	539	315	206	342	334	197	276	292	462
348	651	668	664	246	305	651	258	761	270	466
264	813	510	467	267	347	281	494	377	354	284
308	449	235	430	403	416	182	398	451	547	613
618	598	637	257	628	144	905	615	928	680	576
702	899	929	299	999	189	958	205	262	677	676
262	808	795	765	346	421	226	510	272	493	602
373	267	237	658	619	334	271	185	294	375	546
320	373	242	271	311	261	297	351	274	260	257
288	257	412	477	430	403	443	461	443	431	378
411	517	363	679	665	380	629	460	658	640	642
385	368	331	617	589	604	225	315	212	318	335
294	323	310	323	361	226	344	371	466	350	335
431	457	222	201	278	289	714	257	258	330	120
310	436	530	264	402	334	324	411	449	263	294
356	190	412	457	280	368	290	299	407	181	475
129	730	175	261	306	15	247	233	501	282	177
424	0	410	186	309	258	336	288	652	672	33
314	122	356	416	284	694	240	403	558	820	495
365	389	296	299	388	187	358	137	518	311	535
170	505	604	441	534	289	185	400	270	215	598
256	616	695	336	219	226	637	379	629	120	709
268	874	141	866	257	415	829	214	833	346	654
595	664	204	645	304	323	276	372	246	628	576
457	335	333	787	827	672	390	540	586	342	367
196	363	507	493	585	493	297	408	504	463	632
415	350	552	489	483	506	513	557	321	554	401
469	425	220	488	525	149	596	221	591	603	597
263	414	313	417	306	363	272	391	303	341	

1908.3_1344EC04	197	230	160	262	233	133	216	265	218	217
280	181	150	186	194	164	190	196	223	247	143
230	176	223	172	193	172	172	202	138	227	118
142	127	152	185	162	232	196	145	176	220	269
203	192	150	185	110	222	199	306	189	170	179
351	188	154	133	201	203	166	252	152	225	167
225	179	219	167	230	297	181	201	266	276	225
280	245	271	188	225	285	352	140	228	241	112
180	125	125	156	102	351	156	177	188	198	168
206	143	160	175	189	999	202	252	197	205	214
223	153	149	154	270	169	153	228	245	227	124
175	154	239	198	165	184	239	206	313	235	208
272	258	177	255	168	188	217	109	246	98	167
254	164	260	273	256	255	254	266	222	263	291
283	165	197	165	171	357	182	213	200	223	203
248	222	164	196	191	179	276	161	105	204	217
184	44	189	116	195	142	346	185	234	209	187
197	169	269	156	135	216	189	287	209	196	245
150	138	141	147	202	120	110	235	221	166	178
150	160	176	203	168	231	208	137	131	168	157
61	179	79	129	146	166	131	182	147	132	111
195	168	189	194	193	119	334	157	118	127	12
232	203	190	250	161	160	187	200	189	120	255
119	138	150	197	132	224	258	171	200	198	135
114	223	82	160	238	221	216	189	229	72	207
171	163	157	203	211	141	97	129	82	272	141
139	95	186	99	172	180	117	191	146	202	168
145	164	185	142	176	315	197	225	176	121	193
189	4	165	175	104	134	205	221	207	301	257
198	218	199	172	123	181	123	139	146	196	193
150	239	210	183	206	150	270	187	161	178	196
151	230	78	99	215	136	94	229	154	120	194
221	106	293	279	298	315	296	346	322	188	

1908.5_1185EK16	291	324	219	331	305	287	318	217	690	237
244	308	307	371	416	491	302	316	430	372	365
405	237	491	261	266	460	345	291	662	364	664
666	681	398	446	713	267	646	337	335	303	316
270	301	554	324	237	350	331	215	279	283	444
348	640	643	642	264	293	633	258	751	286	458
284	796	511	453	275	338	286	485	374	345	272
291	445	238	430	400	390	191	409	448	537	612
621	593	620	261	627	141	940	606	934	655	567
678	935	982	260	958	202	999	196	258	654	654
281	783	773	746	322	431	194	523	249	503	574
375	273	210	648	609	332	295	189	314	373	555
304	376	235	244	275	254	256	327	269	280	238
300	264	424	472	441	412	449	464	452	425	364
410	500	359	671	657	386	623	438	647	636	630
373	340	335	596	582	597	210	324	176	325	333
314	333	314	332	335	205	346	337	444	325	353
434	471	147	197	279	318	708	237	252	333	127
324	448	522	254	391	344	320	414	414	269	299
387	205	422	473	255	401	283	299	414	181	482
170	721	177	256	298	140	280	235	508	303	211
413	0	416	212	310	246	336	298	642	660	29
311	121	343	411	264	678	261	391	555	806	484
362	384	306	293	381	185	364	141	508	304	528
171	488	610	423	528	289	183	406	274	204	583
229	607	708	322	214	301	618	367	602	155	704
266	881	176	885	254	434	814	224	815	329	642
597	644	199	676	313	302	278	366	237	665	580
454	239	324	766	826	682	347	526	582	317	351
210	360	512	494	569	498	310	425	489	470	646
411	360	518	499	479	511	507	531	309	532	404
455	419	182	499	502	128	599	241	579	601	586
261	406	317	409	302	373	290	392	318	327	

328

1914.2_2011EC35	291	323	236	308	308	329	299	218	241	236
197	298	753	287	181	226	286	180	163	353	327
344	187	282	571	244	229	592	353	275	323	243
279	262	198	210	258	285	313	395	317	329	197
204	658	301	265	217	232	276	251	337	712	252
289	249	237	243	247	274	241	303	231	269	207
311	231	246	211	288	228	689	224	143	193	223
209	191	462	217	225	249	209	258	173	223	203
195	200	218	177	213	243	218	245	221	257	205
259	221	199	369	205	252	196	999	497	253	251
259	214	215	234	299	232	204	204	309	203	262
207	175	146	238	259	230	327	899	295	352	241
325	322	200	191	224	463	338	258	261	217	201
330	481	219	214	230	245	204	213	237	294	227
183	167	139	239	229	235	231	187	228	221	246
191	330	232	217	233	219	231	160	222	158	207
171	251	170	199	371	205	336	170	228	341	288
292	207	230	818	334	299	255	235	210	312	147
702	174	258	256	199	269	202	287	322	306	326
257	570	321	369	299	181	373	391	215	107	263
201	261	181	245	314	203	206	464	269	297	201
210	309	221	159	271	292	299	276	229	240	25
216	213	288	238	279	236	280	288	266	231	274
273	142	322	292	253	603	204	444	178	264	242
670	266	241	247	243	182	448	196	313	138	293
169	217	272	246	616	109	211	242	215	235	282
119	166	297	180	494	274	212	183	212	306	253
217	249	679	242	155	275	401	272	740	262	210
278	169	743	261	197	302	599	440	367	273	299
213	254	328	235	238	188	235	232	203	211	265
240	196	232	227	204	249	357	214	266	250	206
213	247	149	233	233	263	268	255	242	230	212
221	236	298	323	286	301	331	334	335	245	

329

1916.6_1164EK04	355	336	201	413	386	309	356	177	311	302
301	322	537	460	293	312	344	254	273	340	384
389	228	355	499	309	287	464	400	314	459	284
315	300	278	273	274	172	337	407	343	412	418
549	548	377	308	195	433	505	282	326	633	308
342	257	262	256	393	345	255	290	255	255	243
292	267	247	243	309	249	556	228	263	205	525
238	230	538	265	238	316	199	368	257	288	229
241	252	253	343	256	197	292	315	281	273	248
288	267	247	214	262	197	258	497	999	289	287
206	252	254	253	342	244	274	293	266	290	228
214	300	168	269	252	229	238	499	262	362	266
274	337	271	231	412	566	190	375	335	289	198
258	587	235	243	256	268	243	279	280	295	278
212	209	264	270	268	226	271	242	252	264	257
237	161	190	258	286	268	214	201	145	186	219
210	211	189	154	196	213	294	231	229	181	387
339	285	147	535	312	356	342	149	291	359	158
540	251	285	255	253	335	313	322	399	253	357
299	572	332	380	425	285	484	429	260	161	279
361	318	251	394	425	282	548	543	346	364	190
262	0	289	281	417	516	318	403	298	282	195
336	108	394	281	302	310	382	381	304	285	294
214	280	328	349	259	577	249	399	230	524	241
463	318	258	185	283	243	493	273	286	278	425
202	287	298	219	725	181	282	220	254	143	302
280	236	138	260	948	232	249	219	256	360	318
286	258	621	299	207	257	439	255	536	324	261
258	58	553	305	275	412	451	465	433	278	299
236	241	408	237	295	217	232	244	215	221	350
263	206	281	389	411	288	357	278	228	275	298
276	257	71	251	271	182	285	120	299	294	277
268	220	298	302	282	298	241	309	302	272	

330

1920.6_2011EC41	298	301	199	326	321	315	307	248	603	231
275	391	293	367	416	426	253	442	436	385	424
462	257	510	287	263	507	350	341	502	429	478
496	487	507	550	787	245	715	398	387	302	386
250	345	637	362	219	373	368	285	296	313	617
328	641	652	688	298	379	648	320	768	281	468
306	786	472	474	252	461	273	489	376	379	325
369	536	255	474	371	496	225	411	515	619	716
693	632	682	252	696	160	643	669	658	885	602
887	639	642	263	677	205	654	253	289	999	994
355	648	662	730	348	585	257	521	359	523	640
619	295	293	690	703	593	293	232	375	463	660
354	382	240	355	328	195	278	342	304	296	274
336	210	436	457	452	438	441	496	447	466	496
492	596	505	672	683	516	649	582	712	655	689
494	312	315	664	605	627	223	451	228	447	464
429	440	434	457	304	320	421	483	580	340	348
475	405	173	209	288	307	641	238	125	390	165
267	430	564	271	493	353	419	466	474	377	282
309	193	275	359	321	407	360	334	423	261	569
213	776	231	294	360	96	260	253	590	363	230
468	2	471	278	388	340	369	351	638	701	136
268	177	415	505	341	716	186	464	598	812	622
329	322	198	306	431	244	386	189	628	331	711
179	538	662	421	633	276	263	402	293	211	655
317	731	636	313	195	273	737	479	679	145	628
370	574	160	602	270	493	705	204	718	369	788
684	774	222	649	387	331	240	367	294	640	717
447	163	359	646	612	635	361	518	628	354	309
247	352	585	553	687	571	301	455	627	453	560
515	445	686	553	562	493	521	699	398	525	491
622	477	199	524	666	162	602	262	649	659	687
391	532	377	432	406	406	314	453	355	342	

331

1921.2_2011EC40	294	299	184	324	319	312	307	249	602	232
273	385	289	369	410	425	254	445	436	373	406
464	260	508	294	269	501	347	344	495	429	472
487	480	516	549	787	226	711	397	362	302	389
252	344	642	365	215	377	364	299	303	300	620
326	643	654	690	300	371	649	320	770	279	456
307	788	458	461	251	456	271	476	375	379	329
367	538	248	480	390	507	253	417	500	620	719
694	632	686	255	699	176	642	669	658	885	601
888	639	640	256	676	214	654	251	287	994	999
360	630	646	731	346	586	252	524	368	525	644
620	279	296	697	710	601	301	230	375	461	668
360	388	235	356	331	214	267	347	293	292	270
342	217	437	459	453	440	442	498	449	459	495
493	598	506	672	683	508	648	585	698	653	678
498	288	312	666	606	629	221	434	224	435	449
425	461	424	454	290	320	434	483	581	317	349
471	395	173	207	291	307	641	241	125	383	167
265	426	568	237	511	345	420	458	472	376	271
306	217	286	351	322	404	354	329	434	227	564
183	775	232	271	329	97	262	247	568	369	227
468	2	470	279	380	333	367	346	638	702	159
275	176	411	507	341	718	213	463	595	812	620
328	322	196	323	435	255	387	203	632	334	715
177	540	653	420	631	272	255	420	286	200	658
302	731	643	310	198	266	740	481	682	165	627
369	557	175	586	268	493	704	180	718	367	785
685	776	228	647	384	328	247	364	293	637	725
446	163	356	628	594	634	360	512	624	351	312
248	344	585	546	689	571	302	456	628	454	560
515	444	694	543	543	496	513	677	398	524	488
619	480	189	524	665	173	602	266	649	660	688
394	526	377	429	414	410	322	467	375	345	

332

1924.7_1164EK03	227	232	0	248	235	254	208	220	365	128
215	269	213	294	229	262	157	226	228	289	244
321	223	411	234	272	268	301	235	347	308	319
348	327	310	378	361	0	334	235	232	279	182
265	253	337	235	213	320	276	252	270	237	366
303	303	302	292	250	202	282	316	342	257	313
303	347	339	321	243	305	238	330	258	290	268
259	243	217	269	516	415	283	197	270	332	291
285	314	289	195	294	230	313	328	295	319	310
316	283	267	112	262	223	281	259	206	355	360
999	293	309	328	301	304	236	270	635	283	302
289	279	394	341	339	307	544	255	316	292	276
870	302	196	446	226	165	100	281	292	298	146
564	174	273	315	333	302	267	372	402	442	316
264	271	298	327	325	335	311	295	322	379	334
366	0	223	308	343	349	292	313	229	423	340
340	245	355	337	54	298	319	404	303	0	249
262	275	177	213	203	208	392	225	126	245	164
221	258	305	218	278	247	228	316	375	292	163
275	160	241	323	277	289	199	191	302	250	372
151	343	160	183	247	115	257	225	316	240	218
282	301	309	165	239	232	302	209	309	323	240
260	183	224	319	256	331	157	278	348	357	350
192	301	190	227	224	217	318	108	273	285	323
168	317	287	217	326	249	167	266	212	0	320
219	319	309	235	210	167	290	235	297	225	304
285	235	230	312	209	286	312	233	335	305	316
293	339	203	298	235	262	151	231	279	281	295
264	75	242	316	272	320	148	269	305	261	233
308	231	257	280	347	271	303	249	249	253	271
233	240	274	346	273	333	378	306	133	286	242
295	261	175	304	337	135	309	169	329	331	310
227	236	299	288	324	340	284	362	310	218	

333

1927.7_1288EC32	257	232	118	315	311	243	325	234	598	211
256	300	259	294	367	387	273	284	327	337	343
390	216	429	238	263	387	272	308	514	357	510
501	505	384	483	705	165	619	282	320	255	310
278	295	571	305	179	307	269	199	264	254	457
301	617	650	654	253	277	615	292	750	259	418
301	787	473	424	260	290	236	461	359	329	263
339	412	228	497	341	428	188	418	451	550	667
653	545	634	278	615	111	812	561	841	635	523
635	813	823	111	808	153	783	214	252	648	630
293	999	979	852	307	399	211	513	292	520	644
412	307	260	754	705	377	258	221	274	361	554
316	304	273	284	243	158	101	275	280	224	220
274	153	435	471	456	438	453	471	440	471	431
474	551	359	658	673	382	640	516	684	654	673
403	155	316	636	571	590	219	392	275	427	394
385	399	422	434	151	268	311	408	506	142	315
328	407	101	200	233	325	621	216	167	291	105
283	387	483	253	321	329	354	356	378	305	213
247	148	223	319	256	349	212	229	327	217	474
205	658	87	216	281	41	272	206	511	289	203
400	0	430	256	273	259	303	284	570	649	31
242	167	316	367	279	655	202	384	540	794	490
320	343	327	230	434	188	331	64	551	269	577
147	495	643	423	534	255	174	319	177	216	564
293	626	682	286	179	297	689	346	677	120	672
412	798	125	817	207	374	966	201	943	337	589
572	706	191	663	224	238	191	318	224	662	578
397	195	298	857	893	745	405	525	601	271	232
165	323	535	550	574	513	294	437	487	457	529
409	395	480	540	506	516	422	548	270	455	436
513	399	195	502	591	189	532	126	568	562	565
293	413	264	316	276	308	251	334	235	270	

334

1931.1_1288EC35	258	234	64	316	312	244	325	237	603	211
254	300	260	300	366	387	274	286	310	342	344
386	214	433	239	269	383	271	307	512	361	511
498	503	391	489	713	78	622	284	334	258	313
280	292	558	306	178	308	270	197	262	254	453
303	631	667	670	254	286	632	297	767	260	420
305	801	477	428	264	297	236	466	359	333	261
344	413	227	490	340	432	189	414	455	561	682
667	555	647	278	627	111	801	567	830	645	534
645	802	812	70	795	149	773	215	254	662	646
309	979	999	872	310	406	213	514	291	521	632
413	306	263	764	709	370	259	221	278	367	563
315	312	279	288	244	156	64	275	280	225	209
274	152	439	478	462	440	457	477	444	462	435
479	564	367	664	679	388	644	528	698	657	686
415	96	306	653	585	603	221	398	279	440	402
376	411	434	445	91	263	312	420	519	86	316
329	410	106	200	234	325	626	219	166	292	102
283	386	483	237	327	331	356	359	372	288	215
247	148	223	322	256	353	218	223	339	217	480
205	664	87	219	300	47	272	204	498	289	203
404	0	434	256	274	257	305	285	572	660	13
235	170	327	369	278	669	199	394	549	808	497
300	343	326	221	451	188	331	68	563	267	573
147	493	646	427	547	255	173	331	161	219	572
293	631	682	285	180	309	706	350	695	104	670
399	787	129	807	206	377	965	202	955	336	598
577	706	193	663	227	234	182	308	225	661	586
396	196	299	841	877	747	411	529	603	268	229
166	316	541	548	580	521	302	439	495	461	530
412	399	492	552	519	520	420	561	275	450	436
528	403	195	514	604	181	537	129	585	575	584
299	423	268	310	277	309	253	335	236	274	

335

1935.5_1288EC36	270	236	55	332	325	255	333	249	616	231
261	305	269	303	359	370	285	317	342	352	360
431	229	464	243	281	373	284	331	491	410	483
479	481	406	501	788	103	690	308	361	276	333
281	297	568	331	180	322	289	211	282	258	478
326	746	757	756	296	306	752	328	874	273	443
336	881	476	459	277	350	249	456	359	379	271
377	420	230	460	351	456	205	397	467	649	804
788	658	807	299	784	113	758	592	787	761	636
759	757	768	101	765	154	746	234	253	730	731
328	852	872	999	346	433	217	506	341	513	581
438	289	292	737	688	421	277	217	308	380	636
332	335	294	325	287	144	94	312	278	262	196
289	155	449	553	461	441	471	485	448	453	436
502	617	403	649	663	427	638	551	764	643	746
456	121	299	691	602	616	225	441	291	520	450
427	472	511	533	113	312	318	505	526	119	329
330	387	126	191	243	333	633	242	170	300	94
280	372	471	235	319	333	376	370	417	274	221
248	142	227	331	306	331	238	252	318	260	505
236	715	87	219	307	56	271	218	545	316	216
420	0	464	238	287	230	341	297	594	774	37
221	185	365	378	259	742	183	419	597	893	529
303	359	314	238	461	185	348	71	660	263	621
141	532	692	430	591	259	192	359	177	214	631
298	653	651	284	181	293	819	396	815	149	642
398	672	117	705	234	374	899	221	911	369	662
602	698	187	689	301	229	178	305	234	669	640
437	219	325	743	758	744	462	539	654	267	230
181	301	652	539	608	587	323	448	607	480	555
425	393	595	604	561	518	407	628	299	483	462
549	458	205	481	610	183	547	142	620	605	629
317	462	254	315	277	295	254	325	236	280	

336

1939.9_1185EK11	321	328	230	476	365	328	375	263	426	369
202	377	352	431	260	290	341	260	314	363	528
582	201	393	396	234	288	387	709	308	658	321
320	318	298	337	377	263	349	373	498	366	181
255	343	402	680	249	300	334	287	267	323	303
770	337	353	353	335	350	350	215	363	256	285
228	370	319	291	241	335	320	310	284	304	322
255	280	305	217	338	275	239	226	276	328	344
357	321	353	287	344	261	323	314	345	377	323
372	326	319	232	346	270	322	299	342	348	346
301	307	310	346	999	276	225	263	359	260	274
244	214	202	313	319	242	321	278	325	329	270
364	292	196	295	330	243	218	538	272	316	187
329	277	266	257	280	268	230	271	259	335	229
252	291	234	311	310	303	326	288	332	307	323
301	215	235	289	326	322	206	242	73	249	253
245	232	231	253	232	200	318	229	253	206	467
400	346	312	332	345	375	443	289	321	408	103
333	218	324	256	272	333	452	339	612	265	252
301	243	333	388	595	298	304	435	345	146	342
219	342	218	190	496	156	234	224	314	667	234
227	356	252	203	371	319	737	299	302	367	83
258	135	396	330	299	370	224	385	325	365	329
211	250	271	269	290	320	269	178	397	305	294
210	340	342	294	297	317	326	275	326	96	413
202	290	343	255	275	204	346	282	336	269	278
148	250	386	273	322	339	309	292	330	944	363
273	345	306	330	333	286	270	272	334	345	271
357	139	300	329	279	330	267	301	338	299	322
255	258	361	332	308	293	227	253	320	190	287
209	240	318	299	274	261	381	307	249	300	244
260	261	95	276	301	158	337	223	305	323	263
190	241	274	286	307	322	307	323	303	254	

337

1940.3_1288EC07	256	272	225	275	282	259	340	238	373	283
276	312	304	336	326	351	301	357	339	318	292
367	289	354	275	292	354	298	300	413	317	391
423	407	326	386	486	281	458	309	325	305	250
225	310	429	229	174	252	250	200	303	275	492
274	470	490	484	258	305	479	306	473	322	437
315	476	475	427	322	265	244	443	272	308	242
270	343	273	412	317	401	170	301	380	372	438
443	363	467	322	453	140	434	464	424	518	382
535	430	427	233	421	169	431	232	244	585	586
304	399	406	433	276	999	242	415	295	415	571
899	244	261	480	614	777	263	188	274	366	466
344	317	224	305	344	237	221	347	229	172	209
274	234	323	391	337	374	338	359	380	438	411
327	418	304	502	500	390	460	443	468	477	469
346	239	230	417	490	497	172	353	246	316	389
358	315	315	328	197	298	326	386	428	251	273
449	351	179	272	248	340	391	229	232	307	155
296	354	450	253	400	361	299	395	372	343	245
423	250	418	418	275	312	273	324	334	183	415
214	507	145	243	312	32	230	269	407	239	151
412	0	374	232	318	243	294	282	420	510	23
289	128	339	345	295	437	233	287	381	473	423
268	358	223	246	341	234	382	154	403	285	469
196	396	376	267	451	254	216	314	205	218	446
233	500	437	208	213	222	459	329	433	170	400
410	407	145	415	225	423	431	229	442	283	510
465	534	219	440	268	255	248	261	301	419	484
353	75	304	413	360	360	267	342	380	246	276
189	242	395	300	460	386	281	344	444	352	430
340	312	387	332	318	343	373	463	243	397	333
434	356	198	429	461	152	446	164	487	480	432
213	374	298	351	284	333	201	350	302	249	

338

1940.4_1344EC27	295	328	123	281	292	291	318	92	284	187
186	291	222	283	157	232	269	170	149	316	207
289	256	278	254	207	299	297	232	309	310	289
320	295	291	252	256	107	244	334	340	303	168
227	218	281	183	306	319	303	223	305	240	227
235	210	223	220	221	303	211	213	260	259	255
227	236	230	251	223	199	182	227	207	180	314
218	212	242	211	208	243	207	219	165	244	182
171	228	181	281	185	166	240	271	216	256	218
255	188	193	177	226	153	194	204	274	257	252
236	211	213	217	225	242	999	182	230	182	197
215	318	189	190	208	219	237	199	122	286	172
289	345	224	215	368	318	173	246	338	291	185
230	364	238	204	232	228	251	297	261	234	178
224	180	154	252	254	190	247	200	240	236	223
234	91	227	242	278	284	226	158	37	184	141
147	35	140	150	129	154	262	195	221	85	268
255	121	117	172	266	318	274	108	223	346	86
151	172	251	77	184	221	212	241	311	209	470
232	228	376	364	307	233	285	319	267	127	222
389	193	197	325	331	202	195	257	254	185	277
142	0	165	175	278	272	204	201	263	225	161
309	0	326	209	243	245	244	291	220	267	279
209	207	102	298	166	321	211	134	213	297	146
216	187	248	149	235	169	234	144	167	218	292
103	207	362	250	249	2	212	200	201	111	321
11	208	228	211	267	185	201	54	210	220	284
232	194	287	277	226	254	236	268	220	290	147
176	5	153	245	251	247	169	234	266	241	282
211	264	257	183	296	191	250	152	169	215	259
215	215	200	272	260	244	327	248	75	216	175
226	255	218	216	257	220	242	66	256	267	231
164	184	265	268	272	233	251	246	231	267	

339

1946.4_1164EK02	302	299	159	257	270	306	270	270	683	221
297	351	330	398	536	483	241	363	503	308	327
328	244	460	283	303	437	322	235	635	275	610
652	648	427	515	556	219	550	320	290	245	289
268	360	513	275	220	324	248	231	260	276	409
262	420	429	432	248	277	421	327	502	304	438
300	516	491	447	277	370	264	479	449	344	271
321	403	292	390	367	453	208	386	382	439	419
426	443	448	306	473	140	529	485	506	453	429
453	500	501	283	510	228	523	204	293	521	524
270	513	514	506	263	415	182	999	295	993	495
441	186	152	496	494	367	276	219	310	400	417
319	356	233	221	221	233	249	262	196	189	312
288	212	326	359	329	305	322	337	323	421	324
360	395	328	486	485	357	484	401	520	486	535
342	296	315	463	439	455	247	310	258	350	308
307	292	324	318	331	206	402	330	405	313	266
430	388	181	177	279	270	661	288	167	391	209
342	435	474	340	447	343	275	509	394	315	296
327	231	281	386	192	446	346	295	443	167	496
188	575	233	277	278	69	272	227	465	273	179
472	0	414	281	338	210	253	270	505	449	80
289	170	315	549	317	513	191	380	546	526	477
398	340	298	303	400	265	363	203	370	295	440
214	499	465	366	399	332	258	397	264	229	476
379	456	473	345	238	332	430	289	411	168	465
214	488	196	503	262	531	540	225	546	282	536
433	543	270	429	414	307	230	365	274	428	462
328	190	289	511	494	497	176	432	445	330	303
187	359	387	433	411	409	265	286	320	319	495
326	314	440	408	412	360	498	475	279	472	357
390	351	167	469	451	175	396	245	426	432	445
323	403	357	380	381	409	358	441	364	301	

340

1947.0_2011EC48	219	285	143	285	298	274	260	247	322	156
270	298	263	268	251	248	230	228	169	307	264
331	255	362	227	226	288	274	302	269	317	285
261	265	270	338	376	169	354	246	289	332	278
227	267	338	263	226	302	262	284	296	245	401
318	319	301	304	331	211	298	289	345	252	306
270	338	309	315	251	331	259	311	260	302	261
259	274	270	258	632	364	268	233	282	326	301
303	269	324	149	297	230	268	336	271	356	268
358	255	241	230	272	245	249	309	266	359	368
635	292	291	341	359	295	230	295	999	293	281
299	309	556	356	346	308	369	286	342	292	269
660	301	247	605	299	204	228	257	295	310	209
395	199	257	302	274	278	254	320	322	382	305
265	248	216	286	292	327	280	259	351	309	328
312	199	184	282	280	288	324	414	197	517	434
443	282	490	427	209	414	371	550	300	233	266
274	239	245	191	285	260	324	240	124	344	137
238	201	281	192	221	244	239	292	360	179	229
228	193	250	260	233	254	263	281	215	143	316
257	307	166	156	269	218	219	220	283	265	216
211	262	234	223	291	211	304	247	258	297	34
282	145	238	169	239	319	194	253	258	343	338
223	183	162	256	201	244	243	165	267	268	249
155	287	285	213	296	223	238	262	290	183	327
214	291	280	215	241	233	313	273	282	228	325
221	188	291	227	273	247	315	192	314	331	331
308	324	285	323	235	261	197	247	232	284	256
210	121	200	307	227	237	157	196	253	284	250
261	246	252	289	309	252	258	187	244	242	213
212	240	279	289	244	260	343	274	200	255	230
241	289	201	227	282	142	247	245	269	251	275
231	206	344	353	321	383	348	397	375	260	

341

1957.4_1164EK02	303	298	161	255	269	303	275	268	681	246
296	347	329	399	537	488	260	363	486	293	323
326	246	459	280	293	449	314	232	634	269	609
653	650	424	518	563	225	547	315	290	236	283
263	364	518	272	221	322	243	228	267	276	411
260	422	427	431	247	274	424	322	509	314	430
298	522	484	441	291	365	265	472	448	347	271
325	404	290	393	368	450	207	385	382	444	427
432	444	455	308	480	127	511	490	488	462	435
462	482	481	269	493	227	503	203	290	523	525
283	520	521	513	260	415	182	993	293	999	498
432	186	155	503	496	371	277	218	312	379	424
330	359	229	224	226	231	243	269	193	189	303
286	218	314	367	318	294	313	330	312	421	327
360	406	332	489	490	364	487	409	526	491	542
345	288	311	472	445	461	252	310	257	348	307
307	291	324	318	323	207	406	326	413	306	266
429	390	178	177	275	275	658	288	200	387	206
321	439	474	352	450	341	275	508	393	327	286
323	230	285	384	183	448	338	292	442	167	502
186	584	225	273	278	69	267	224	463	270	179
468	0	420	275	339	204	251	272	507	447	80
314	170	313	547	317	513	225	410	556	530	468
395	361	302	305	411	263	366	217	377	292	453
207	510	476	379	402	337	264	397	258	228	476
377	464	490	342	236	349	438	286	418	143	468
214	492	164	501	257	528	548	222	553	277	539
438	544	270	433	409	306	233	361	273	433	470
351	191	291	515	500	494	175	446	451	326	295
182	355	389	429	408	413	264	272	333	307	498
327	315	429	406	413	359	495	477	293	477	364
399	359	178	451	454	145	409	247	436	440	448
314	412	366	383	372	417	358	445	378	300	

342

1959.2_2011EC40	260	271	289	277	287	228	267	239	498	229
312	307	277	327	446	455	260	396	392	349	277
382	261	428	223	226	402	314	262	410	334	433
420	428	376	442	518	323	567	294	301	266	321
315	331	613	274	187	376	316	159	244	252	588
268	499	480	484	264	277	480	300	554	218	402
268	556	409	400	231	320	273	388	382	301	276
294	360	248	447	353	462	175	394	435	466	453
478	420	460	269	490	125	579	500	583	568	426
576	575	536	316	602	124	574	262	228	640	644
302	644	632	581	274	571	197	495	281	498	999
647	298	238	792	839	660	227	223	271	371	509
291	307	301	281	285	166	313	279	314	226	201
268	189	360	393	370	363	365	440	399	467	452
375	457	349	562	564	399	511	465	521	531	539
376	335	249	516	499	504	257	390	155	381	402
406	356	379	379	344	304	320	378	483	317	287
437	391	182	178	213	267	522	198	155	306	219
258	375	633	249	421	328	286	382	375	412	169
303	94	287	328	246	389	271	219	341	197	402
185	562	60	247	272	16	300	230	575	261	155
404	0	415	252	266	230	276	286	475	488	24
177	141	293	334	215	510	131	317	427	611	374
318	388	252	314	290	193	324	94	437	260	634
97	423	548	357	436	273	169	331	194	153	472
287	492	490	235	176	253	502	286	469	62	540
18	604	162	632	208	443	641	218	655	284	529
444	807	172	540	313	254	190	246	268	534	541
312	136	342	697	619	554	230	429	439	267	259
210	240	437	481	495	421	286	312	470	357	490
331	365	466	430	434	393	375	498	273	510	422
417	354	183	398	513	125	452	102	486	486	495
275	400	283	365	255	279	170	294	220	268	

343

1961.3_1288EC07	237	257	239	233	247	261	277	231	409	213
228	301	272	318	340	363	230	372	344	286	250
348	250	351	227	261	339	307	257	414	316	400
425	408	310	430	492	290	487	295	267	275	258
195	293	492	211	182	267	252	208	245	232	576
239	449	539	522	230	271	521	287	466	281	404
299	435	417	406	278	273	226	402	268	288	228
288	323	245	377	300	392	160	306	397	394	451
454	396	413	232	457	185	413	447	402	499	371
516	389	373	244	373	175	375	207	214	619	620
289	412	413	438	244	899	215	441	299	432	647
999	241	233	566	709	873	242	194	208	355	460
299	326	179	279	288	218	248	306	204	172	194
254	235	297	360	296	343	311	348	372	433	385
307	406	312	469	460	379	426	436	466	447	466
317	274	250	397	468	461	174	282	220	285	329
292	291	292	296	221	284	332	341	426	244	245
445	366	167	239	249	277	428	234	183	282	144
284	369	518	248	427	315	246	381	376	425	227
384	235	360	397	269	292	254	263	348	185	450
158	513	151	222	264	28	219	214	471	220	121
356	0	333	212	274	231	248	253	430	480	16
288	137	306	358	232	429	252	302	421	493	407
306	306	203	236	328	202	365	201	404	296	579
176	390	404	272	427	250	206	283	216	207	448
234	481	439	230	189	256	483	325	466	159	407
398	438	115	460	221	437	420	230	455	274	502
450	606	208	431	267	243	253	262	288	409	470
341	72	295	432	413	367	259	362	388	233	303
192	250	371	311	438	356	261	301	418	297	442
344	341	410	337	337	347	385	452	267	413	353
420	335	204	412	452	126	431	131	464	450	412
210	364	307	366	303	344	209	362	313	259	

344

1975.9_1344EC27	237	283	141	290	280	228	225	170	243	208
180	263	203	296	208	260	183	251	233	246	198
327	269	299	252	242	294	235	251	265	358	262
286	267	239	237	232	136	245	293	262	347	236
255	313	249	196	220	353	275	235	255	266	247
217	188	224	210	328	290	212	249	260	195	263
225	262	293	240	200	195	226	256	186	234	310
217	194	261	235	273	277	198	185	212	304	197
202	269	204	317	246	181	345	260	344	208	270
208	339	331	173	267	154	273	175	300	295	279
279	307	306	289	214	244	318	186	309	186	298
241	999	199	301	277	214	251	136	137	298	218
277	324	217	200	342	364	136	327	769	737	196
273	335	240	230	233	275	232	225	285	272	210
214	269	194	303	288	168	276	263	271	276	269
208	138	242	274	301	286	219	204	69	193	195
160	205	141	152	183	173	297	190	261	140	284
266	204	142	205	224	225	259	226	193	283	116
183	199	241	216	273	271	197	277	335	248	291
269	210	354	330	320	254	286	288	244	64	237
300	244	189	280	283	64	247	238	290	188	185
198	0	254	235	294	290	228	283	305	234	187
344	146	309	241	268	252	270	314	265	269	244
260	263	190	284	237	271	258	184	225	307	195
169	255	285	218	244	253	243	233	235	211	362
228	231	266	264	282	88	221	160	225	282	275
15	315	216	328	326	231	296	186	326	237	272
223	292	270	341	255	266	294	287	237	353	274
270	10	180	346	335	324	173	291	319	253	261
711	284	359	283	291	225	276	260	187	219	283
255	224	250	299	301	288	329	268	117	310	224
266	216	254	286	275	179	312	121	332	307	277
192	240	300	308	327	333	335	299	277	255	

345

1985.5_1164EK03	205	211	164	169	158	210	159	250	333	119
198	281	146	251	183	208	177	208	122	195	172
375	253	372	225	184	219	203	201	249	280	255
232	230	175	237	336	218	328	215	176	288	200
179	180	234	166	200	171	263	224	196	157	309
258	309	303	316	231	125	296	198	303	234	313
182	281	346	318	241	218	189	342	177	262	159
198	177	174	191	398	214	222	217	173	278	275
281	251	293	180	235	175	244	279	251	284	261
282	227	196	207	237	239	210	146	168	293	296
394	260	263	292	202	261	189	152	556	155	238
233	199	999	240	244	192	332	153	268	234	255
478	241	177	963	251	192	226	290	177	197	222
293	166	221	225	235	243	212	228	210	277	212
206	209	170	287	278	202	248	303	313	223	277
229	255	272	244	263	269	255	368	295	432	373
490	279	413	458	208	475	296	488	230	235	177
183	148	208	186	227	159	322	273	117	289	202
114	252	229	245	220	206	193	287	410	191	282
164	186	209	275	281	153	179	216	182	165	269
117	308	205	165	193	178	163	173	210	193	185
204	158	228	158	223	188	257	205	289	284	27
294	219	169	141	226	279	204	266	208	309	203
234	125	116	256	197	199	225	178	275	162	243
149	240	226	193	334	157	191	261	248	118	354
170	303	279	295	206	0	315	264	302	269	307
319	237	280	236	163	136	275	103	284	252	271
325	288	172	257	178	288	182	302	139	247	266
235	101	172	273	236	214	191	201	224	283	282
232	305	187	227	305	183	142	159	218	177	194
121	185	269	213	201	209	360	308	184	254	158
289	213	190	214	333	176	267	216	244	230	294
151	145	289	334	331	332	328	342	307	274	

346

1991.6_2011EC38	276	249	118	345	344	269	318	212	575	292
281	350	285	357	419	393	300	367	452	325	278
454	255	477	269	223	398	306	295	518	385	528
496	494	415	495	634	176	590	334	306	273	353
279	312	726	288	213	335	297	197	264	271	685
314	580	572	576	283	288	567	337	688	250	447
318	706	468	457	264	324	292	449	370	339	265
327	362	249	472	390	461	173	413	478	575	617
640	545	608	237	645	139	665	541	673	702	534
703	659	637	91	658	198	648	238	269	690	697
341	754	764	737	313	480	190	496	356	503	792
566	301	240	999	900	607	257	255	300	401	591
311	350	297	301	284	175	95	326	271	279	228
296	205	334	436	370	337	349	405	368	450	433
421	515	450	572	584	423	541	494	607	557	600
453	107	313	575	517	526	232	443	259	459	450
444	387	441	461	109	304	324	470	506	100	338
427	401	130	259	261	318	602	207	212	351	138
270	362	643	205	439	326	311	449	458	482	255
290	187	249	321	293	381	286	310	367	178	481
201	676	191	269	256	62	279	248	673	305	190
454	0	461	275	296	235	344	303	529	590	41
224	147	319	465	218	655	212	384	522	765	447
317	362	255	258	384	198	341	165	526	279	790
165	475	618	384	512	273	185	418	224	261	547
260	601	583	294	191	250	664	271	630	116	668
360	678	137	678	236	407	765	179	788	349	631
536	903	199	599	314	238	200	320	245	604	617
372	154	384	705	696	658	348	519	574	272	255
214	318	511	536	538	537	325	378	540	391	593
390	379	525	508	484	439	424	578	339	556	407
467	380	173	394	543	196	482	176	540	552	550
292	365	287	355	323	337	165	367	294	286	

347

1997.0_1288EC09	260	251	120	334	340	236	322	214	540	254
282	324	278	329	362	380	268	331	430	352	307
429	241	442	260	201	392	324	304	480	389	473
469	470	384	449	614	165	574	312	327	293	353
288	293	672	288	191	337	295	174	255	276	634
293	588	567	573	294	284	563	333	652	244	439
321	677	463	442	259	308	303	433	333	333	257
303	410	246	461	366	470	177	374	465	541	589
608	500	582	276	612	129	634	546	636	669	512
670	622	605	95	619	165	609	259	252	703	710
339	705	709	688	319	614	208	494	346	496	839
709	277	244	900	999	727	260	263	297	383	553
325	344	282	297	316	144	98	329	261	258	278
297	202	349	419	366	361	361	433	396	456	468
377	488	410	591	602	424	549	484	603	567	608
430	126	301	577	529	542	261	438	256	429	447
410	381	418	443	110	289	315	447	508	128	348
399	372	127	249	242	322	570	202	144	327	123
289	379	593	172	402	328	334	427	422	442	230
277	151	248	342	312	365	267	259	350	160	432
241	636	163	265	281	61	298	247	624	293	186
420	0	444	254	310	249	321	263	531	590	41
214	105	321	417	207	605	166	352	510	723	439
311	391	258	255	353	184	334	149	491	270	727
165	423	552	351	531	260	185	373	211	161	518
266	612	547	266	188	230	626	328	593	138	583
392	608	114	622	211	435	718	178	741	344	610
561	930	186	604	304	234	155	302	298	599	574
371	125	381	672	658	614	324	461	524	244	247
188	299	502	504	561	489	326	393	521	385	517
398	365	487	491	493	433	413	544	299	518	388
452	380	158	427	541	193	497	158	539	560	572
278	371	282	326	299	309	207	332	252	277	

2014.0_1288EC06	256	258	57	266	296	239	284	231	391	209
289	323	293	318	401	383	256	379	376	338	252
329	255	357	241	236	335	309	250	360	292	353
364	354	327	459	470	3	444	259	244	290	321
257	294	534	229	161	305	276	212	283	262	654
238	443	431	435	239	266	429	289	434	244	335
279	418	345	341	260	307	285	336	311	304	218
287	363	222	364	323	401	160	340	428	382	392
426	353	404	246	417	159	340	424	330	538	358
541	325	323	125	334	184	332	230	229	593	601
307	377	370	421	242	777	219	367	308	371	660
873	214	192	607	727	999	229	218	231	321	458
296	284	227	266	267	121	123	274	230	212	171
266	161	258	336	291	311	285	350	351	436	430
307	367	299	414	414	404	380	435	432	419	422
329	87	264	398	408	403	207	375	263	382	394
355	314	350	364	101	303	286	393	416	91	290
433	338	99	252	229	284	407	225	86	326	143
295	368	549	233	406	327	277	397	353	475	208
271	85	258	310	241	338	257	225	332	182	437
235	493	113	245	237	4	295	253	503	236	148
393	0	354	266	252	199	258	236	404	441	0
242	130	273	355	234	449	159	299	396	459	353
286	371	242	240	331	203	348	84	358	257	576
126	336	405	314	402	269	138	303	182	138	433
276	490	341	241	159	304	463	291	405	171	372
340	323	92	348	175	443	413	264	406	283	486
445	670	169	385	267	206	105	245	302	372	482
310	95	287	389	352	345	224	389	368	226	207
172	227	360	351	433	335	246	257	419	284	348
356	299	390	339	317	324	382	436	258	401	379
421	317	149	334	471	213	388	166	410	398	401
214	346	256	276	255	291	200	313	244	218	

2066.6_1164EK03	220	263	40	230	239	202	250	243	325	184
257	246	263	196	170	193	199	180	104	326	263
329	214	293	202	144	229	267	282	314	321	220
301	269	219	240	292	113	280	244	251	302	205
156	211	260	224	236	303	282	289	262	247	277
347	290	273	271	271	190	272	364	282	300	256
323	302	291	258	256	332	244	274	206	264	217
266	218	262	239	329	405	255	212	273	334	248
237	227	269	137	223	255	272	286	274	300	226
287	269	266	199	271	239	295	327	238	293	301
544	258	259	277	321	263	237	276	369	277	227
242	251	332	257	260	229	999	296	304	303	244
613	314	272	344	237	197	189	244	268	212	209
969	198	304	339	315	331	313	387	417	406	352
271	241	230	252	266	319	263	258	284	302	262
401	139	222	224	268	267	325	258	117	316	288
223	57	286	257	162	231	347	355	255	137	238
165	233	267	200	230	250	315	250	79	254	99
214	111	227	49	157	204	143	236	305	147	176
175	149	187	257	284	194	222	266	104	0	216
203	262	134	82	207	115	136	186	219	202	243
129	224	199	129	274	194	336	138	169	311	1
228	191	244	152	203	262	153	230	207	271	315
213	79	218	156	157	239	221	102	173	172	184
182	230	213	172	226	203	256	251	235	0	240
185	172	302	229	212	94	242	224	232	216	276
220	191	213	246	220	239	254	217	276	308	293
241	249	244	290	176	282	92	223	250	259	204
237	3	183	287	234	198	201	133	268	294	291
255	232	215	223	240	255	287	219	199	244	109
122	270	231	320	244	340	356	242	67	135	209
190	328	140	200	293	181	206	205	251	240	211
240	176	310	287	323	311	288	341	340	241	

2075.8_2011EC34	267	295	162	283	300	327	308	245	233	247
186	284	737	270	226	259	272	210	152	338	293
287	167	261	559	234	227	561	350	290	327	248
304	271	222	238	243	166	211	366	331	338	147
177	677	298	253	187	257	240	233	353	766	256
288	267	226	252	253	229	246	336	220	280	206
325	205	237	212	311	257	775	232	181	288	240
270	223	493	217	225	256	170	267	221	254	218
199	219	213	247	181	153	203	258	203	251	211
250	203	192	174	185	206	189	899	499	232	230
255	221	221	217	278	188	199	219	286	218	223
194	136	153	255	263	218	296	999	261	318	277
279	283	246	177	257	449	181	290	206	184	152
271	450	223	226	234	266	220	214	235	280	256
190	202	219	223	211	234	204	202	230	228	226
228	182	221	243	224	207	154	198	86	203	274
218	158	199	227	161	208	322	202	266	174	288
267	196	139	822	315	308	272	287	241	314	194
699	204	279	238	247	288	146	304	290	288	315
246	562	336	365	282	158	380	396	232	141	269
179	258	250	213	332	236	175	479	287	266	186
187	29	263	178	269	253	297	258	235	245	0
213	114	225	286	275	200	252	307	279	211	272
266	197	322	244	239	652	304	478	211	258	273
665	218	229	224	247	293	453	218	234	88	286
168	248	258	237	648	191	216	267	192	206	275
0	166	257	206	492	247	205	193	209	276	232
222	231	775	217	247	220	369	239	755	220	241
292	136	749	243	191	314	587	437	358	217	249
162	236	315	257	269	199	119	225	214	200	278
242	208	212	241	164	245	319	237	152	182	231
250	248	97	210	264	237	278	233	237	218	232
209	238	252	264	238	274	295	300	310	215	

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2086.8_1344EC29	363	277	188	251	247	329	231	251	394	155
196	274	320	334	312	326	179	259	289	352	324
275	215	350	353	211	341	342	314	367	356	364
361	364	314	402	385	172	379	335	261	248	137
193	293	368	256	205	359	237	358	233	274	334
350	306	332	315	207	290	317	330	326	314	256
316	351	287	252	302	284	264	275	288	333	240
299	321	259	248	387	330	325	194	295	331	259
284	280	287	244	273	275	311	354	311	371	285
382	304	284	199	294	313	314	295	262	375	375
316	274	278	308	325	274	122	310	342	312	271
208	137	268	300	297	231	304	261	999	344	315
340	383	230	278	237	269	198	252	228	102	201
310	318	263	315	297	304	240	328	308	378	269
274	263	245	313	311	253	310	276	307	320	302
185	178	191	292	316	300	254	260	164	238	266
287	168	247	226	160	215	368	249	265	193	273
414	326	487	265	334	231	419	256	186	290	128
298	345	368	249	288	307	280	409	360	220	315
407	247	330	382	313	299	280	266	323	123	385
86	431	165	263	334	102	170	299	300	282	190
283	480	257	196	274	234	341	223	361	321	26
304	237	309	325	170	375	263	336	398	377	384
217	307	179	229	296	296	328	191	290	264	332
228	351	255	280	321	318	251	276	337	112	406
182	324	305	256	279	171	333	246	317	275	343
136	281	412	339	283	365	293	200	319	362	394
321	342	250	360	255	306	287	262	285	357	292
297	46	322	308	277	339	323	353	397	310	282
174	246	344	329	307	313	252	283	283	276	376
236	249	313	270	281	291	399	331	203	395	236
291	244	112	307	314	167	326	260	323	342	299
248	240	334	311	304	374	359	376	347	233	

2089.0_1288EC05	325	363	195	370	357	356	357	262	341	277
	340	303	348	423	313	371	364	327	281	393
	405	297	365	384	277	402	381	370	377	319
	389	365	428	385	388	227	421	450	413	358
	260	407	342	312	178	391	342	286	351	404
	307	397	406	406	338	432	403	364	372	397
	332	376	395	406	332	401	375	396	312	336
	338	314	408	370	285	398	248	396	318	378
	379	372	390	380	388	240	396	387	393	391
	460	388	367	235	375	235	373	352	362	461
	292	361	367	380	329	366	286	400	292	371
	355	298	234	401	383	321	303	318	344	375
	327	355	330	269	349	400	221	320	349	249
	319	376	361	391	383	384	360	410	381	381
	326	387	377	424	419	413	413	397	417	396
	445	221	320	407	449	439	266	304	201	302
	283	237	294	274	271	281	389	348	383	335
	558	314	128	316	341	357	359	255	220	182
	314	323	409	253	354	403	260	385	427	336
	378	308	348	358	284	296	415	418	331	406
	314	439	309	263	392	194	260	277	342	203
	315	0	401	300	446	337	306	321	372	123
	264	144	458	378	349	395	284	439	313	444
	309	204	301	347	285	384	296	294	346	348
	263	355	408	232	350	323	387	316	370	472
	257	376	432	341	349	189	397	284	401	463
	297	367	152	342	359	348	378	221	372	478
	365	372	346	421	360	360	311	393	419	402
	344	223	350	409	379	439	356	408	461	379
	272	379	455	383	337	348	289	324	331	355
	317	305	471	408	407	384	401	454	278	368
	413	387	253	375	432	217	386	244	446	352
	375	341	388	441	384	396	285	422	403	334

2091.4_1288EC40	254	242	165	310	296	231	289	263	445	215
227	256	252	282	382	389	258	338	405	330	316
348	224	366	219	203	349	262	264	342	317	347
353	352	404	487	628	231	586	317	271	246	319
240	303	436	259	161	312	264	253	262	280	471
285	582	575	579	228	276	574	317	620	251	369
302	587	386	379	235	371	237	370	246	344	245
346	387	217	452	351	453	234	350	488	517	573
572	525	575	218	573	191	529	507	556	633	516
630	549	537	193	546	208	555	241	266	660	668
276	554	563	636	270	466	172	417	269	424	509
460	218	255	591	553	458	244	277	315	375	999
300	302	269	294	261	130	204	265	224	226	233
269	168	418	461	420	422	441	458	432	475	454
600	496	417	582	573	394	512	534	566	519	546
380	194	301	501	471	490	237	415	293	440	435
393	407	425	454	204	348	357	464	479	220	324
323	329	96	240	221	289	467	252	113	268	120
263	397	352	203	385	350	369	401	348	289	222
290	188	234	271	258	354	247	251	341	142	483
157	547	213	268	231	83	237	234	430	273	131
512	4	428	247	267	243	309	295	451	601	95
219	188	315	368	252	588	169	373	414	615	466
275	309	281	244	349	192	345	197	542	271	517
144	429	530	344	565	258	188	406	228	231	561
283	610	458	287	162	221	598	394	567	221	453
394	478	108	517	246	403	602	211	617	306	540
581	596	202	537	338	229	162	323	203	504	952
373	128	303	537	508	476	248	457	484	241	216
214	314	472	426	522	501	322	422	515	430	384
440	506	575	474	455	452	385	558	315	434	427
500	472	142	360	577	227	487	194	518	496	667
294	415	278	299	303	284	242	330	276	290	

2101.9_1164EK03	205	304	147	283	301	260	284	238	357	166
251	284	273	267	260	253	239	241	220	332	273
360	248	382	234	226	307	303	318	320	360	290
306	289	305	387	372	170	346	264	289	319	255
236	289	309	269	258	359	274	265	287	289	369
342	351	335	327	309	241	329	320	338	240	338
297	351	350	342	247	311	286	337	276	276	281
265	272	284	287	509	399	261	230	303	342	319
322	301	340	158	311	281	325	327	330	375	295
344	311	292	213	320	272	304	325	274	354	360
870	316	315	332	364	344	289	319	660	330	291
299	277	478	311	325	296	613	279	340	327	300
999	335	236	498	305	213	215	290	328	318	170
628	212	280	330	304	316	285	350	367	417	313
315	299	256	303	307	354	301	280	359	351	349
397	190	229	297	311	317	315	388	193	457	405
394	246	434	404	181	353	376	509	311	226	308
279	295	235	192	253	284	358	242	151	317	109
243	181	296	204	222	256	222	286	364	161	231
270	202	245	323	270	253	256	299	210	176	332
222	306	115	167	267	147	231	212	263	266	246
200	240	255	167	285	220	327	253	257	353	22
277	170	275	170	236	305	209	288	296	349	337
225	214	213	266	210	245	216	202	278	276	225
182	296	294	172	276	200	257	314	309	168	334
179	266	337	236	257	199	332	249	301	240	303
259	213	238	279	282	269	330	243	330	332	357
291	301	267	320	248	274	206	253	271	289	276
239	184	234	321	244	260	180	218	297	323	325
294	249	277	247	343	279	306	229	232	272	229
213	275	284	348	291	292	354	287	137	237	273
241	304	188	257	312	153	259	241	295	285	285
255	217	356	371	331	367	321	382	355	260	

2127.8_2011EC19	317	404	171	296	317	371	305	194	329	186
272	294	309	368	257	272	277	211	228	364	277
327	237	391	307	241	319	372	308	360	334	320
381	354	263	289	352	189	319	338	381	351	254
206	318	380	298	287	340	308	335	338	306	325
311	361	353	351	341	347	355	304	331	283	327
274	341	375	333	273	324	304	357	257	254	309
247	275	318	270	348	377	337	291	293	360	321
345	324	334	244	356	226	369	362	373	378	325
388	366	375	199	373	258	376	322	337	382	388
302	304	312	335	292	317	345	356	301	359	307
326	324	241	350	344	284	314	283	383	355	302
335	999	302	304	415	313	185	316	335	330	200
346	342	296	320	299	306	289	337	322	392	306
274	306	229	375	368	339	350	305	338	361	361
315	173	238	318	344	348	257	251	108	246	276
156	118	257	227	180	183	321	276	304	177	285
338	269	227	234	361	305	321	170	178	356	154
256	219	327	194	206	283	178	307	375	299	343
331	221	389	351	278	247	293	365	212	33	304
213	327	123	170	380	112	187	256	301	291	287
257	125	261	199	319	237	277	286	247	365	135
319	135	378	165	259	331	276	277	243	340	357
341	204	207	312	231	330	221	189	266	291	287
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359

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360

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DEMANDE OU BREVET VOLUMINEUX

LA PRÉSENTE PARTIE DE CETTE DEMANDE OU CE BREVET COMPREND PLUS D'UN TOME.

CECI EST LE TOME 1 DE 4
CONTENANT LES PAGES 1 À 361

NOTE : Pour les tomes additionels, veuillez contacter le Bureau canadien des brevets

JUMBO APPLICATIONS/PATENTS

THIS SECTION OF THE APPLICATION/PATENT CONTAINS MORE THAN ONE VOLUME

THIS IS VOLUME 1 OF 4
CONTAINING PAGES 1 TO 361

NOTE: For additional volumes, please contact the Canadian Patent Office

NOM DU FICHIER / FILE NAME :

NOTE POUR LE TOME / VOLUME NOTE:

1023

CLAIMS

1. A method for analysing the metabolites of a biological sample which comprises quantitatively determining one or more metabolites in said sample in a way that said quantitative determination resolves isotopic mass differences within one metabolite,
said method being characterized in that the sample comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.
2. The method of claim 1, further comprising, prior to quantitative determining the metabolites, combining the biological sample (i.e. the first biological sample) with a second biological sample in which the metabolites are not isotopically labeled or are isotopically labeled differently from the first biological sample; and determining in said biological samples the relative quantity of metabolites which differ by their isotopical label.
3. The method of claim 2, wherein the first and the second biological sample correspond to different phenotypic and/or genotypic states of the cells comprised in the samples or from which the samples are derived.
4. The method of claim 3, wherein the different phenotypic and/or genotypic states are different developmental stages, environments, nutritional supplies, taxonomic units, wild-type and mutant or transgenic genomes, infected and uninfected states, diseased and healthy states or different stages of a pathogenicity.
5. The method of any one of claims 1 to 4, wherein at least 50 metabolites are quantitatively determined.

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6. The method of any one of claims 1 to 5, wherein the metabolites comprise sugars, sugar alcohols, organic acids, amino acids, fatty acids, vitamins, sterols, phosphates, polyamines, polyols, nucleosides, adenine, ethanolamine, nicotinic acid, uracil and/or urea.
7. The method of any one of claim 1 to 6, wherein the isotope is ^{13}C , ^{15}N , ^{18}O or ^2H .
8. The method of claim 7, wherein the isotopically labeled metabolizable compound is U- ^{13}C -glucose, $^2\text{H}_2\text{O}$, H_2^{18}O , U- ^{13}C acidic acid, ^{13}C carbonate or ^{13}C carbonic acid.
9. The method of any one of claims 1 to 8, wherein the biological sample comprises yeast cells or plant cells.
10. The method of any one of claims 1 to 9, further comprising fractionating or purifying the biological sample so that the sample contains a subset of the metabolites contained in the cell from which the sample is derived.
11. The method of any one of claims 1 to 10, wherein the metabolites are quantitatively determined by mass spectrometry.
12. The method of claim 11, wherein mass spectrometry is MALDI-TOF.
13. The method of any one of claims 1 to 12, wherein the metabolites are chromatographically separated prior to quantitative determination.
14. The method of any one of claims 1 to 13, further comprising the step of introducing external standards for one or more of the quantitatively determined metabolites.
15. The method of any one of claims 1 to 14, further comprising the step of identifying one or more of the metabolites which are quantitatively determined.

16. The method of claim 15, wherein said metabolites are identified by secondary fragmentation.
17. The method of claim 16, wherein identifying of said metabolites comprises electron impact ionisation, MS-MS technology and/or post source decay analyses of molecular ions or fragments.
18. The method of any one of claims 1 to 17, wherein said cell has been maintained under conditions additionally allowing the uptake of an isotopically unlabeled metabolizable compound and said compound and/or metabolic products thereof are quantitatively determined.
19. The method of claim 18, wherein the amount determined for the isotopically unlabeled metabolizable compound and/or said metabolic products thereof is compared with the amount obtained by carrying out said method correspondingly, but without the uptake of said unlabeled metabolizable compound.
20. The method of any one of claims 1 to 19, wherein, in addition to metabolites, one or more proteins and/or transcripts in said sample(s) is/are quantitatively determined and analysed.
21. The method of claim 20, wherein said metabolites and proteins and/or transcripts are each determined from the same biological sample.
22. The method of any one of claims 1 to 21, wherein said analysing further involves suitable statistical evaluation and correlation analyses of the data obtained and, optionally, network analyses.
23. A set of isotopically labeled metabolites obtainable from a sample which comprises or is derived from a cell which has been maintained under conditions allowing the uptake of an isotopically labeled metabolizable

compound so that the metabolites in said cell are saturated with the isotope with which said metabolizable compound is labeled.

24. Use of the set of isotopically labeled metabolites of claim 23 as a quantitative standard for determining the amount of one or more metabolites in a biological sample.
25. A kit comprising an isotopically labeled metabolizable compound and a manual for use in carrying in out the method of any one of claims 1 to 22 or the set of isotopically labeled metabolites of claim 23.
26. Use of an isotopically labeled compound that can be metabolized by a cell for labeling the metabolites in said cell in a saturating manner.
27. Use of an isotopically labeled compound that can be metabolized by a cell for the quantitative determination of metabolites in a biological sample comprising or being derived from said cell.
28. Use of an isotopically labeled compound that can be metabolized by a cell for analysing the metabolite profile of a biological sample comprising or being derived from said cell.

Figure 1

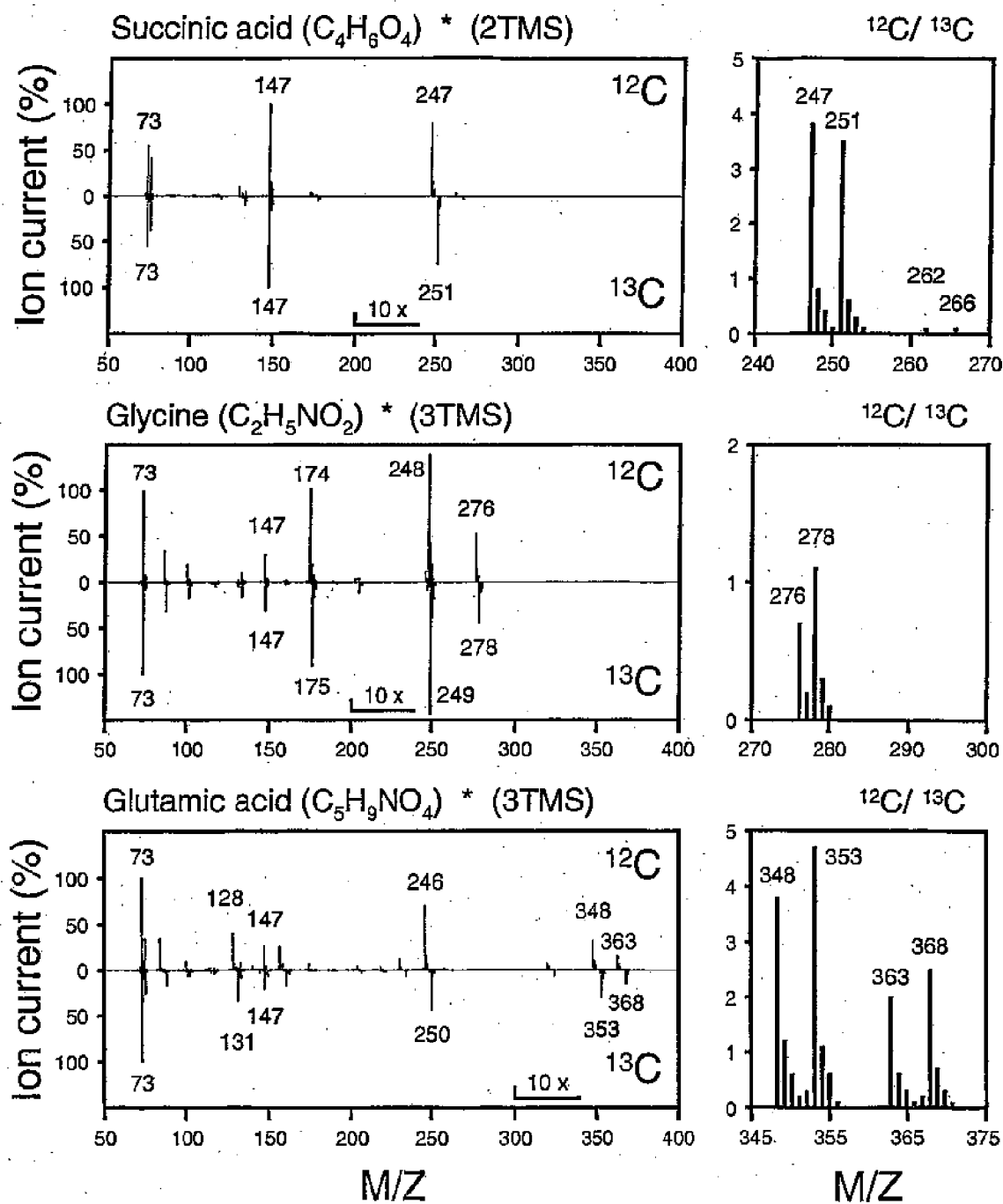


Figure 2B

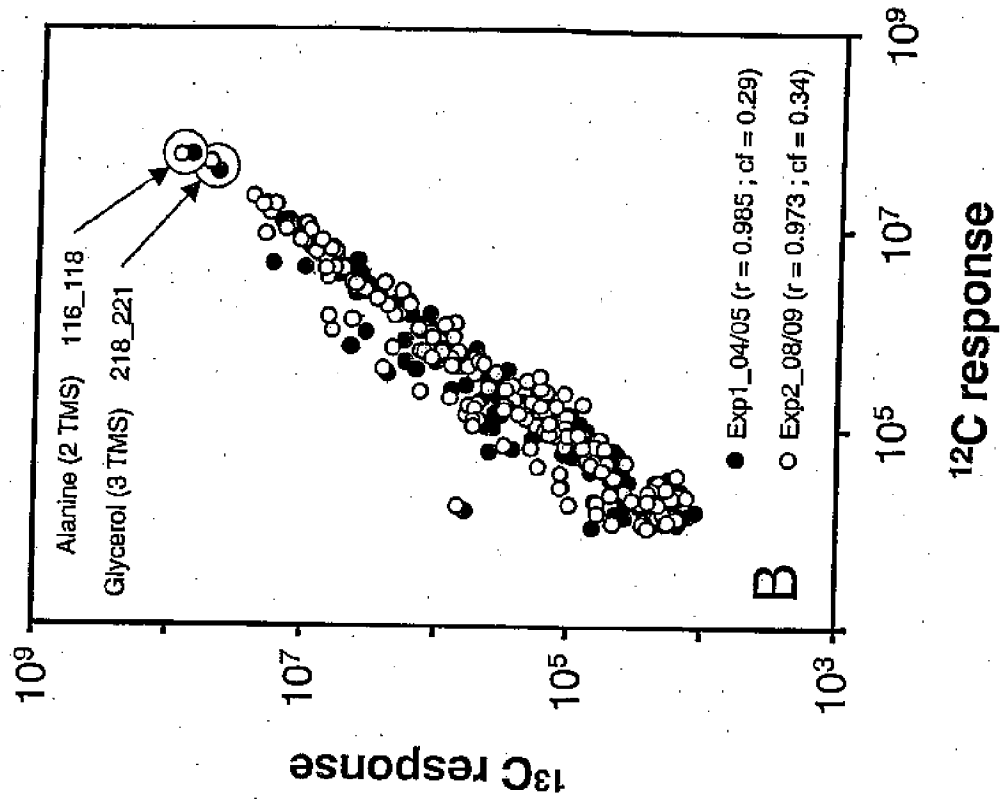


Figure 2A

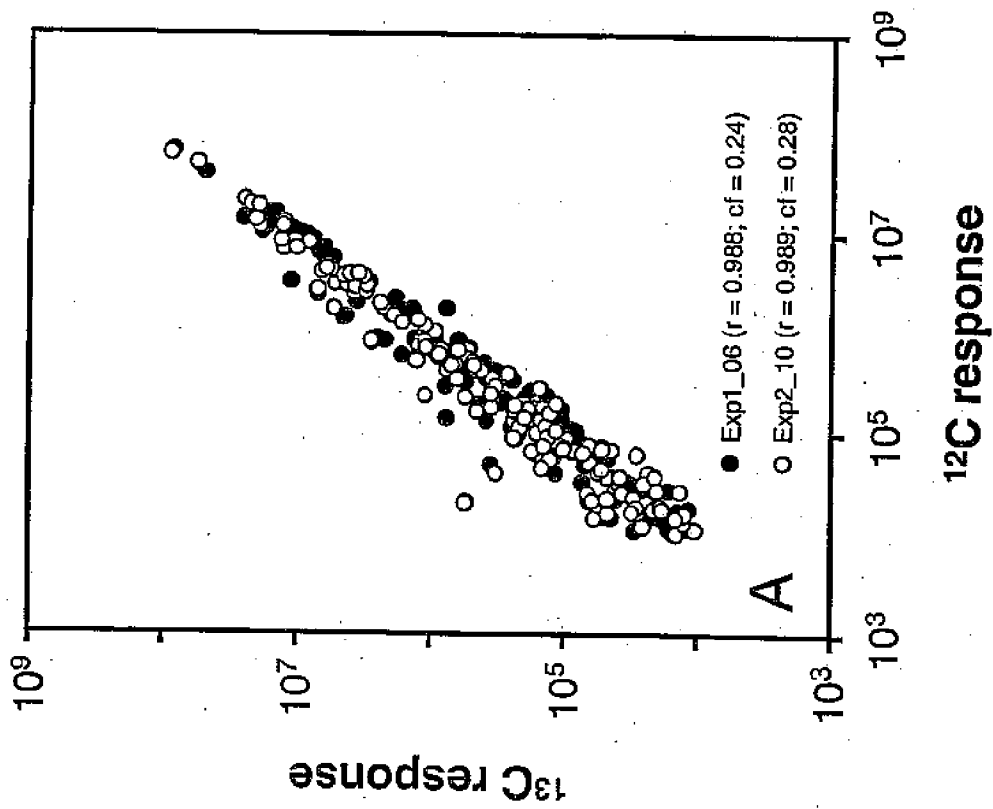


Figure 2C

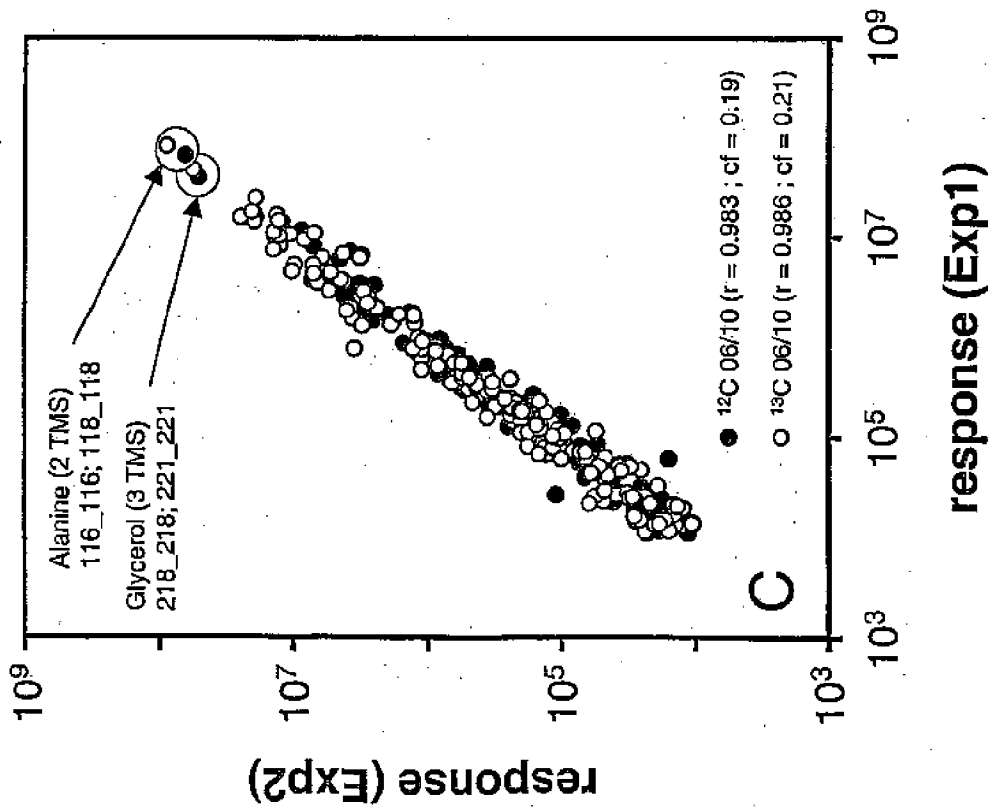
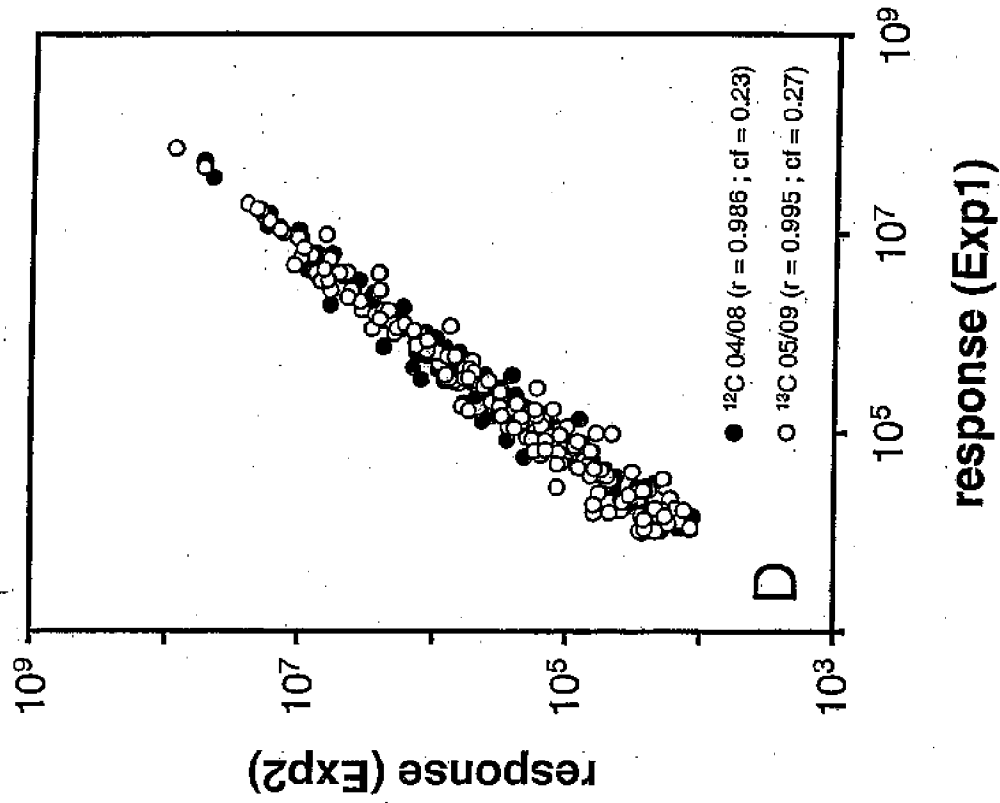
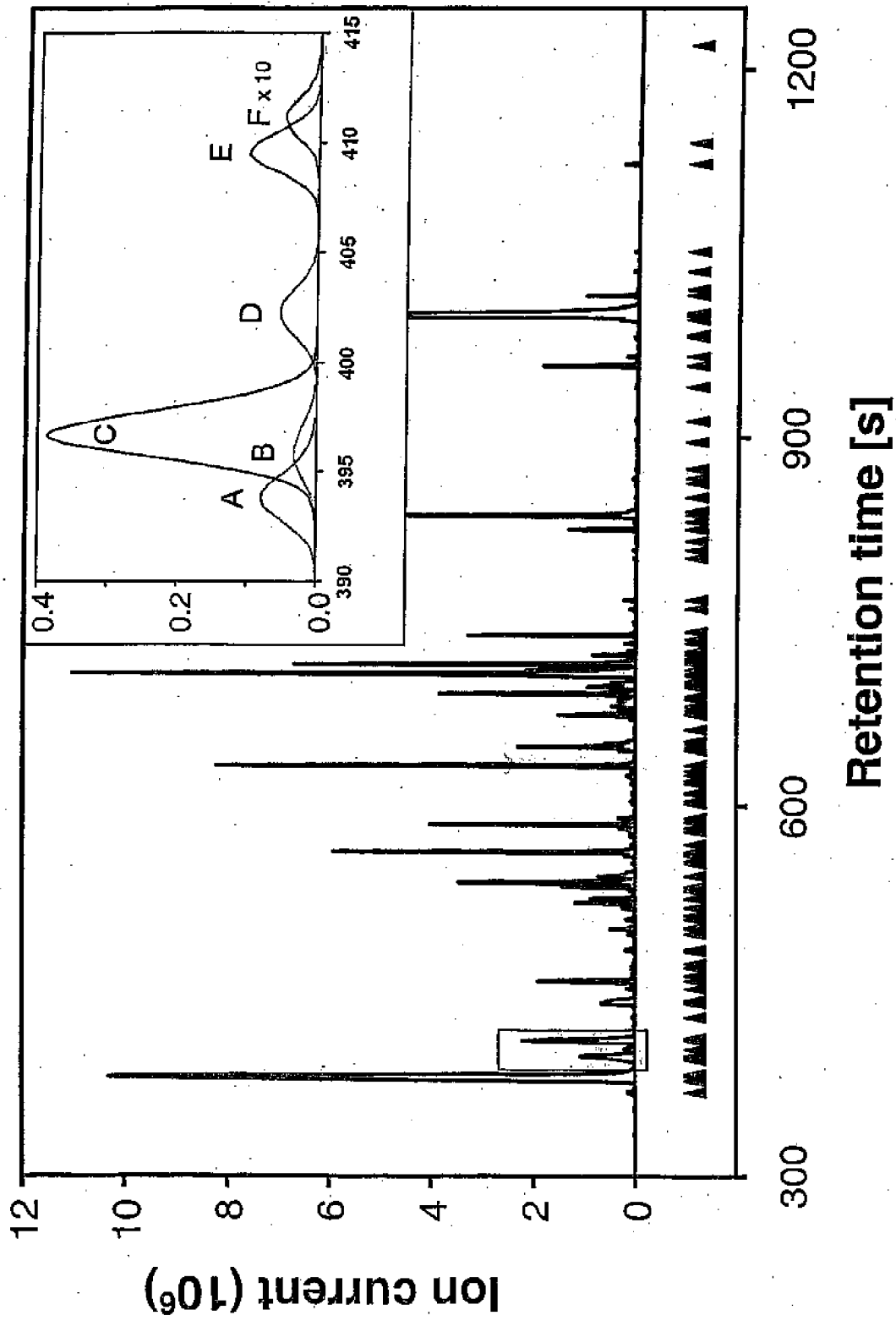


Figure 2D



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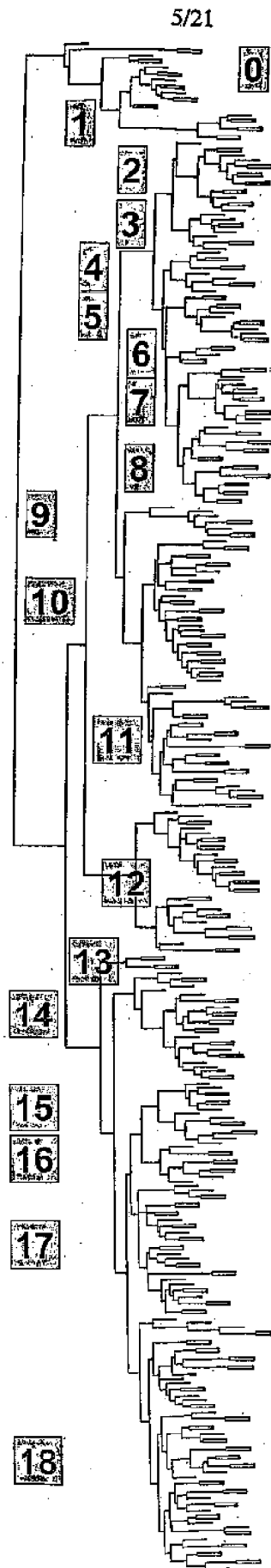


Figure 4A

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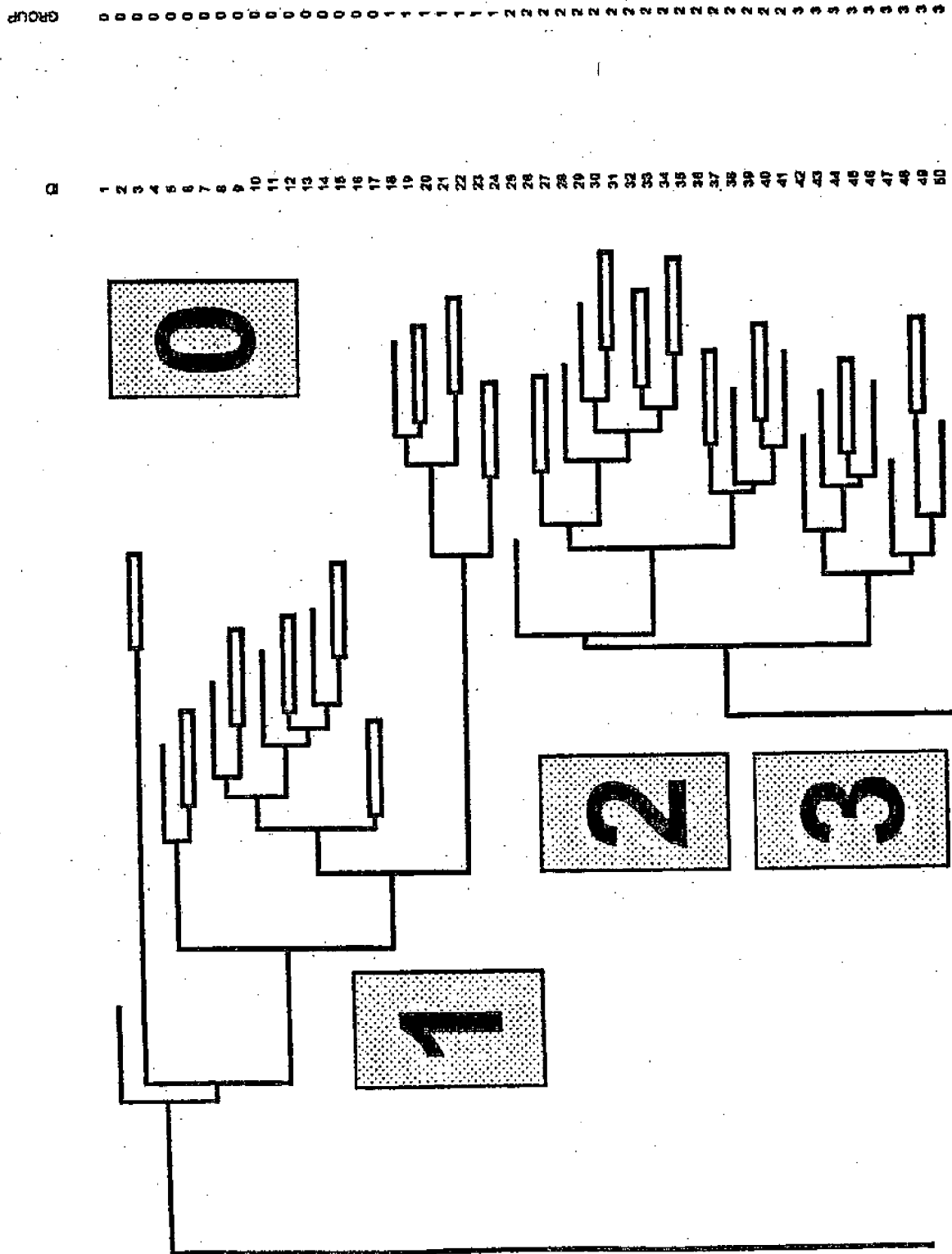


Figure 4B

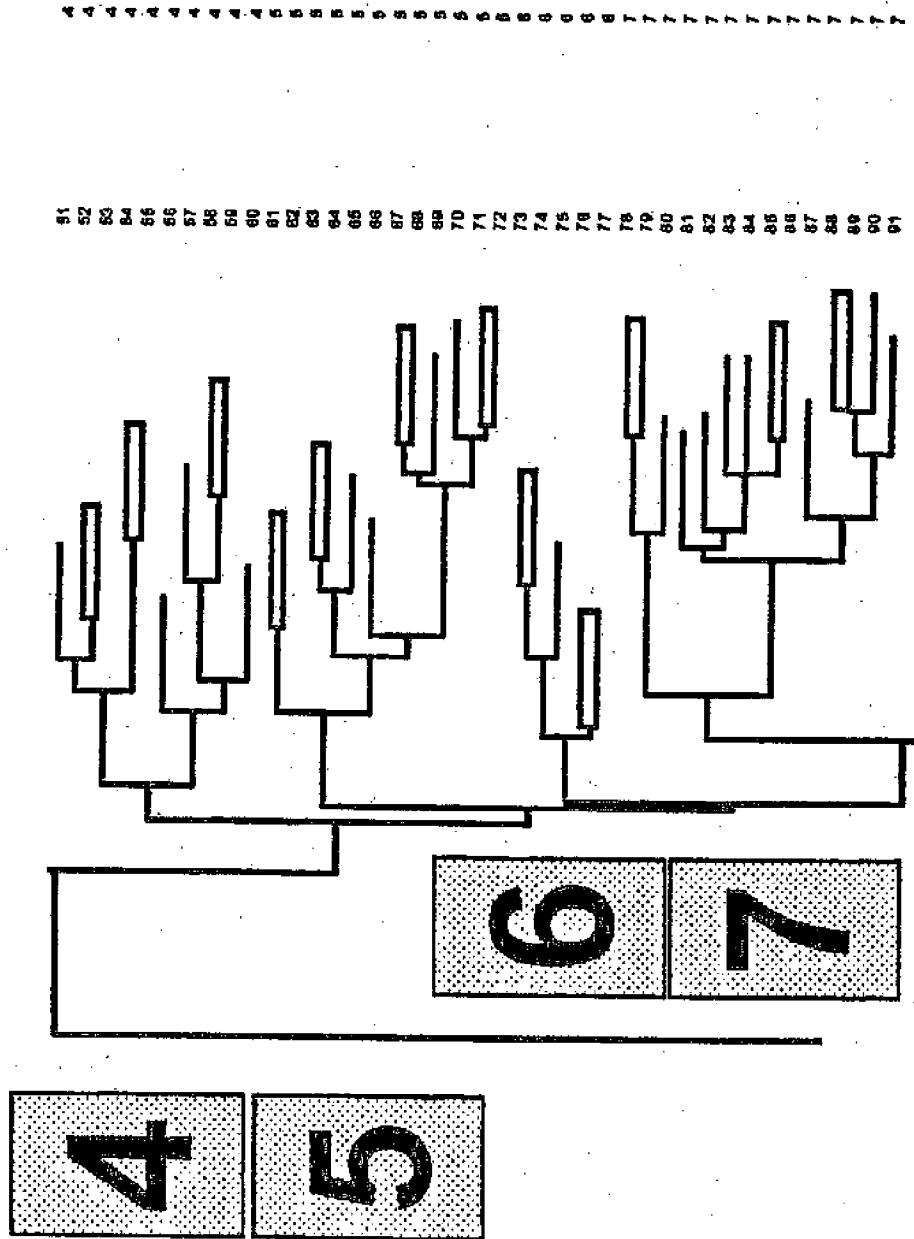


Figure 4C

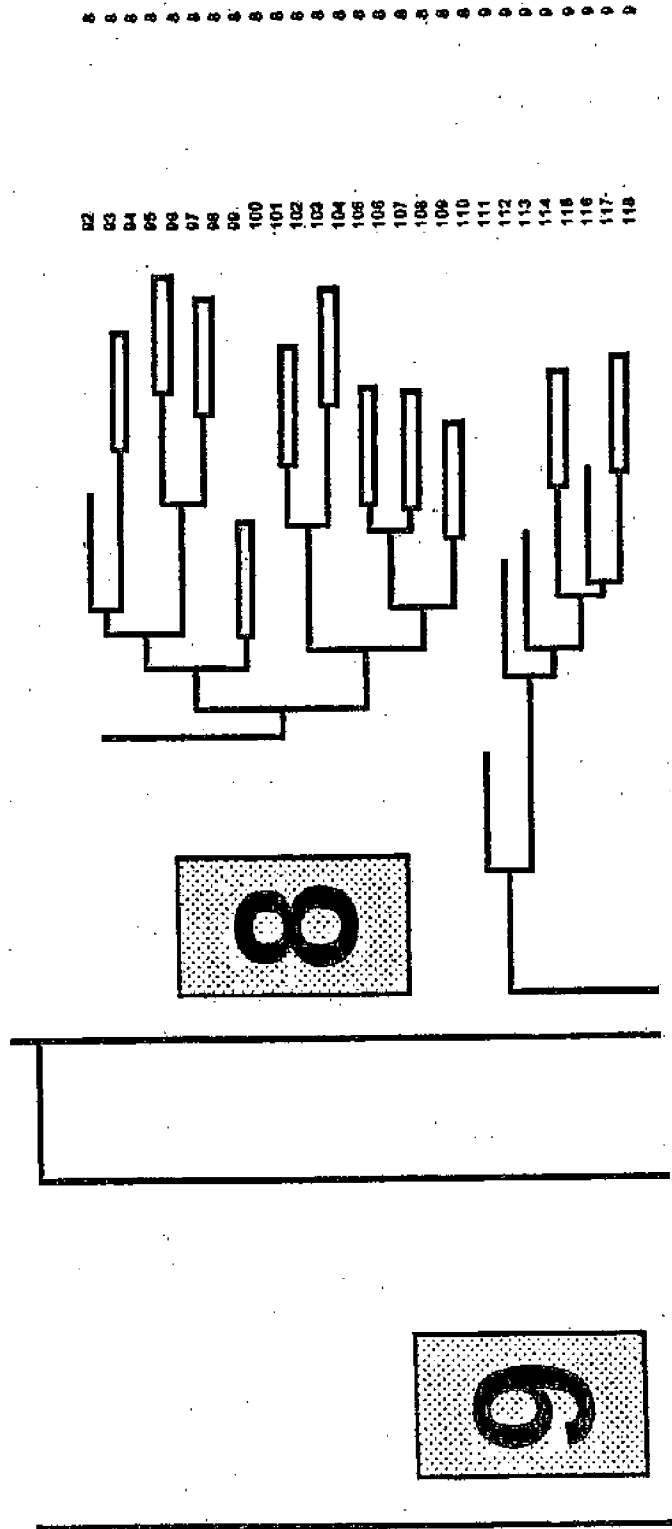


Figure 4D

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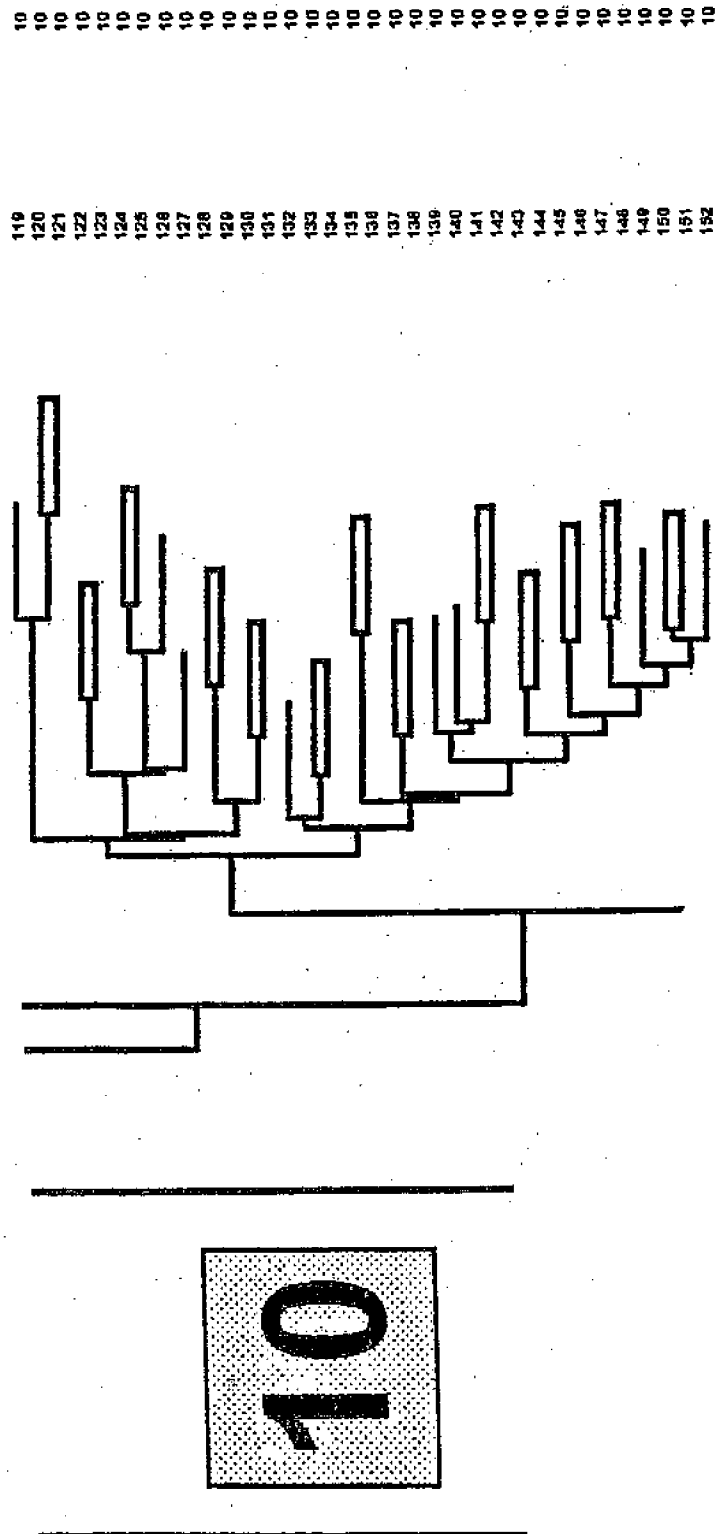


Figure 4E

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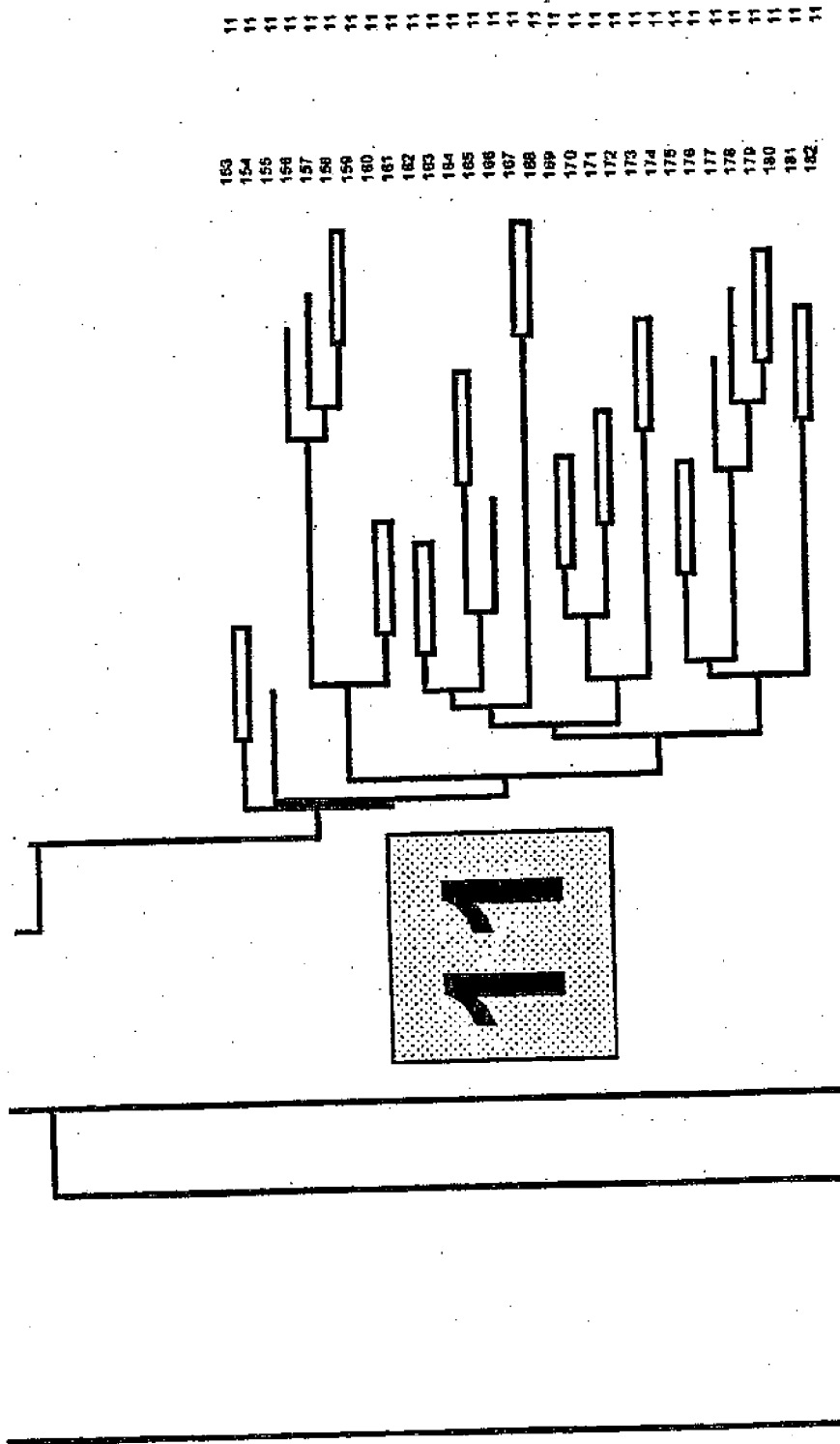


Figure 4F

11/21

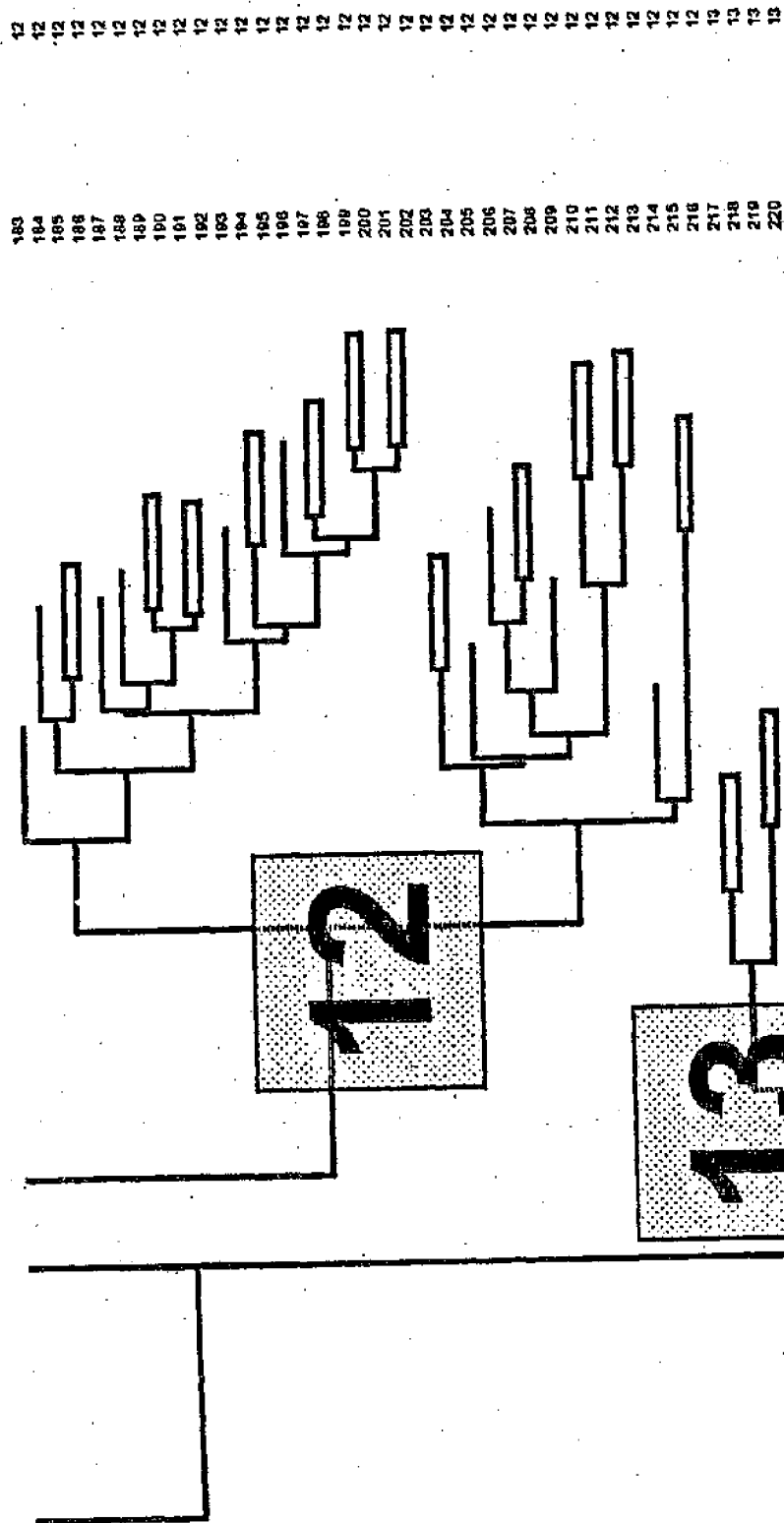


Figure 4G

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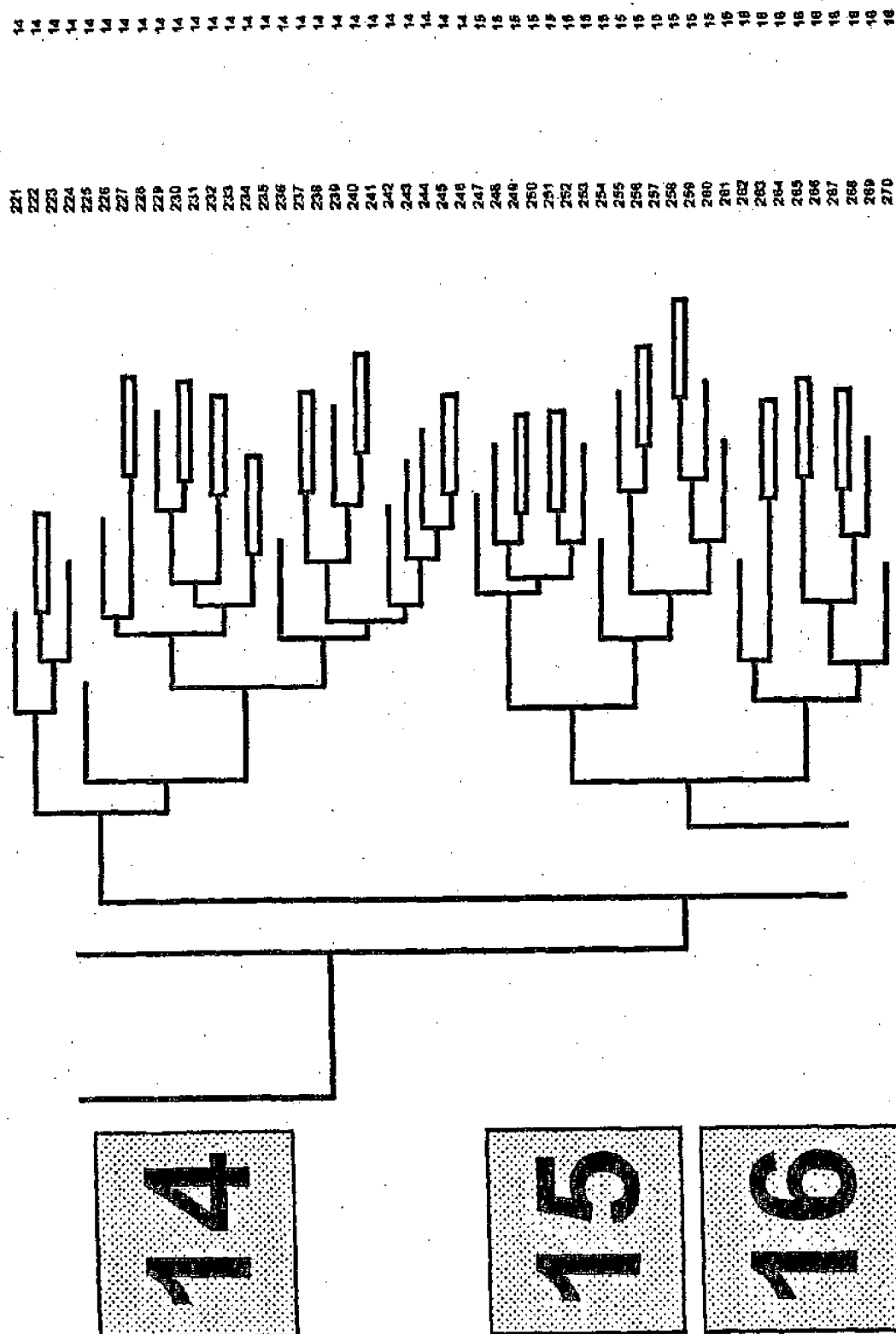


Figure 4H

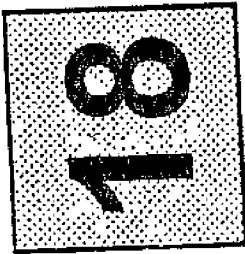
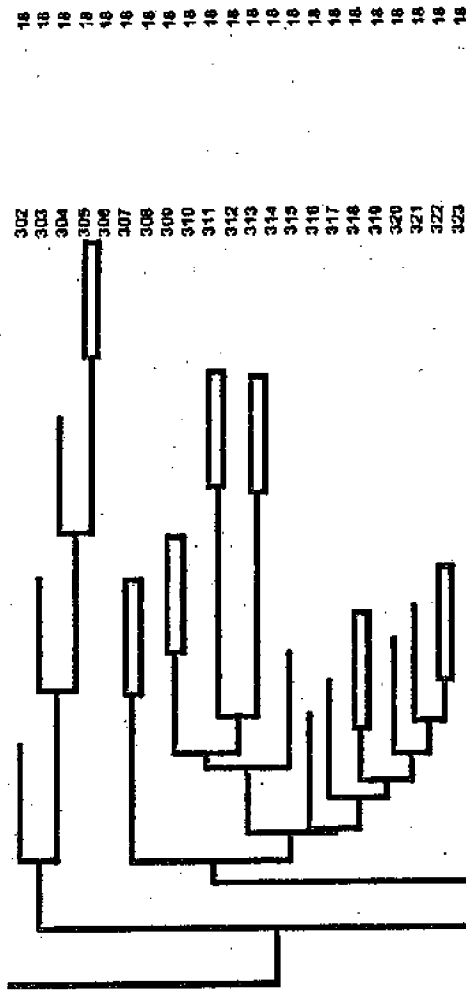


Figure 4J

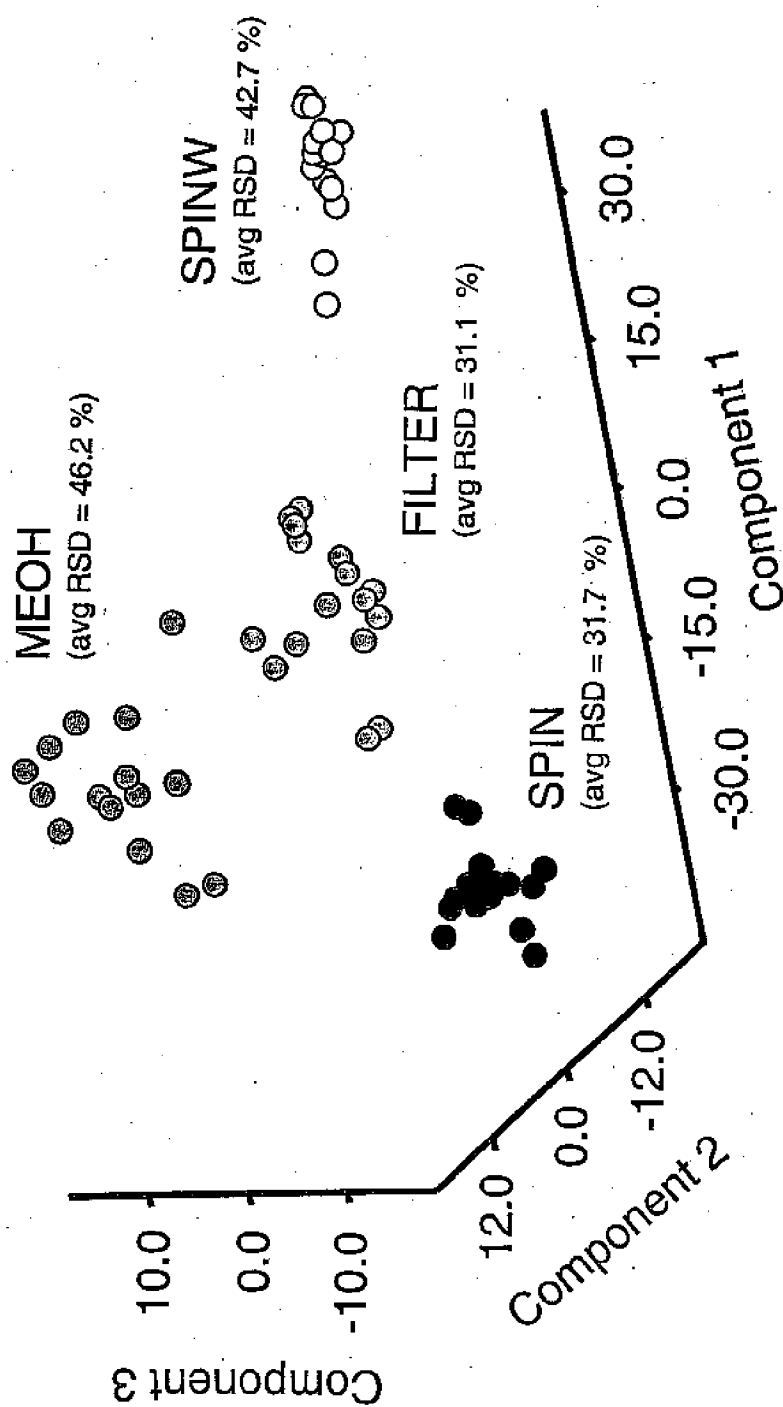


Figure 5

Figure 6

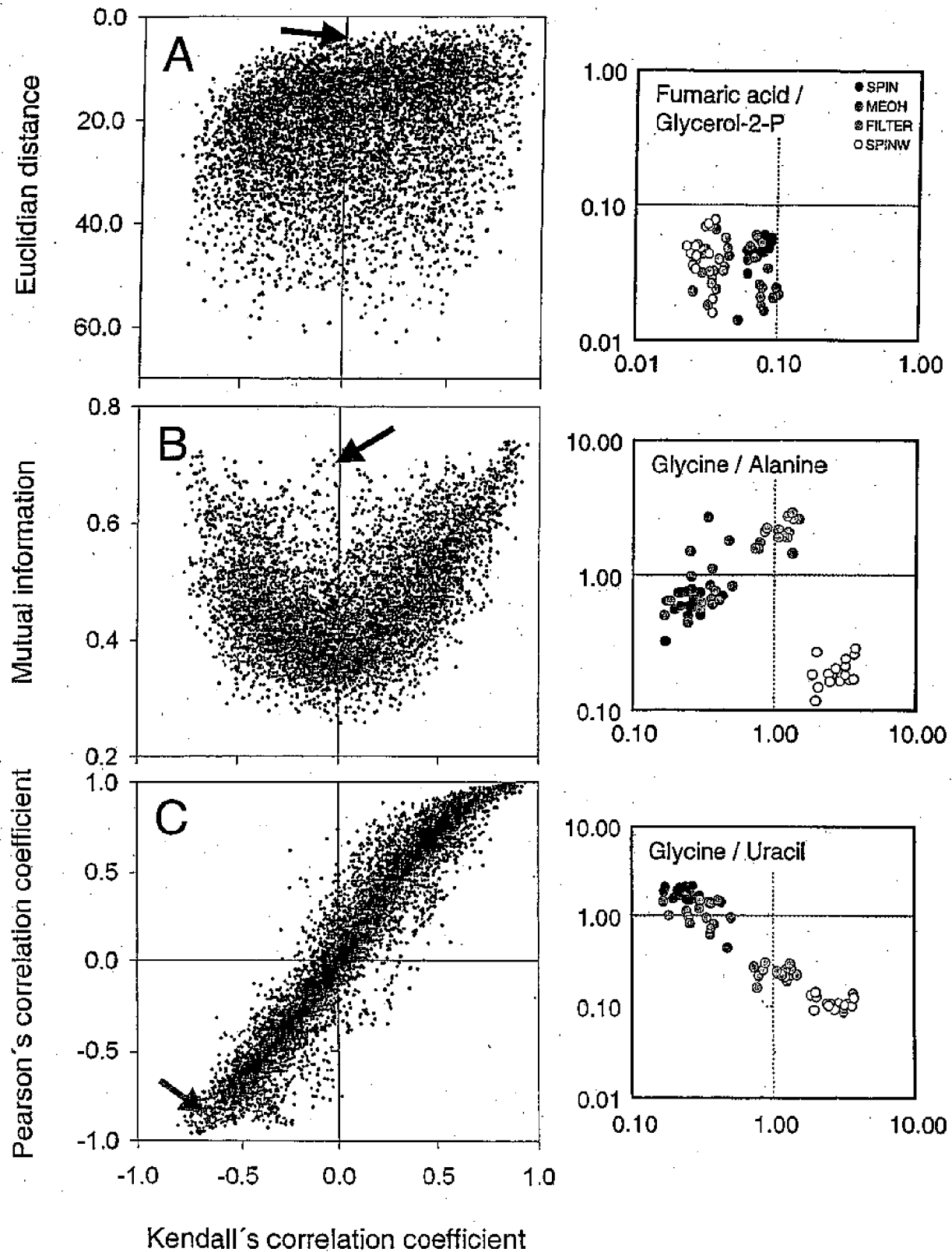


Figure 7

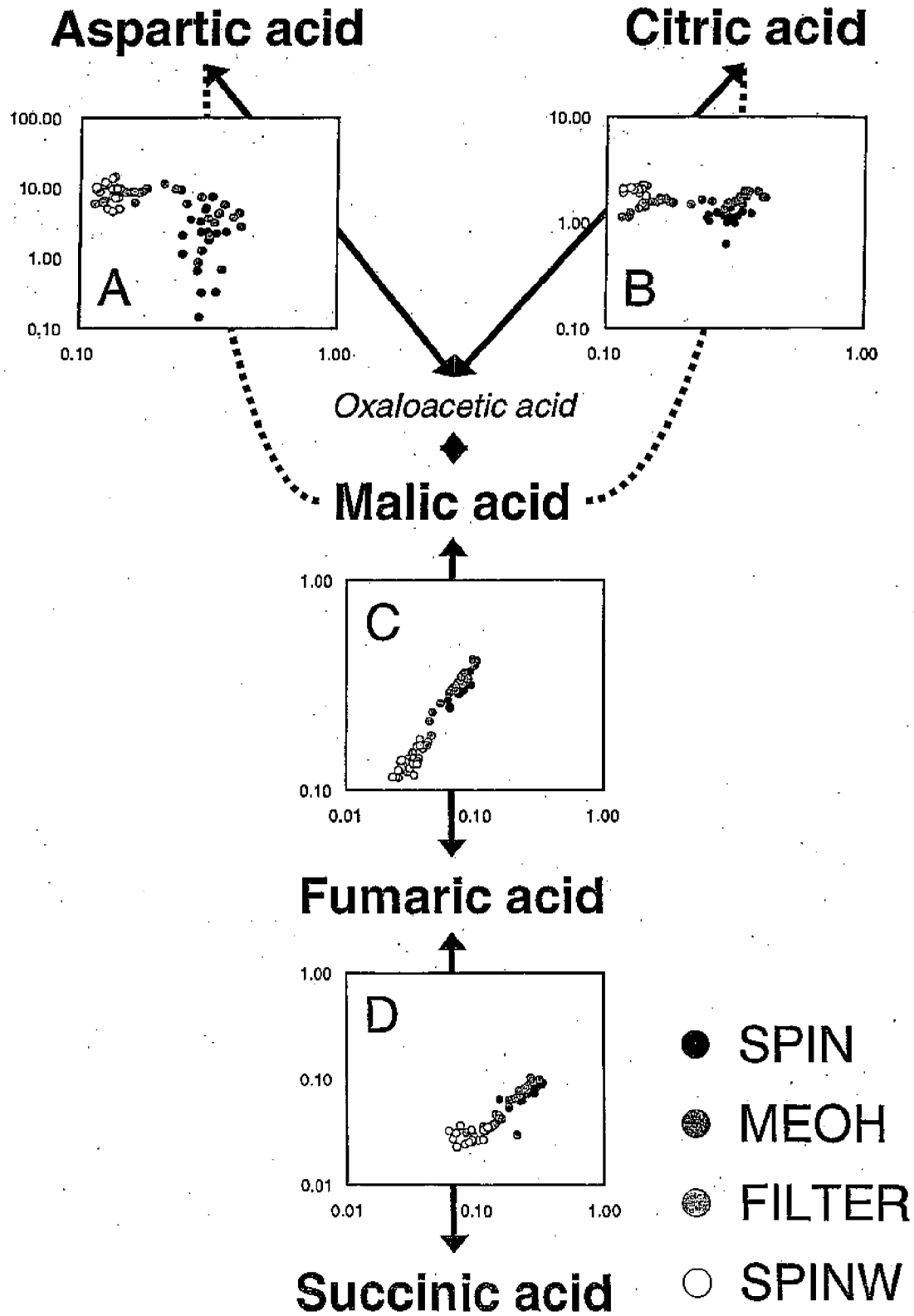


Figure 8

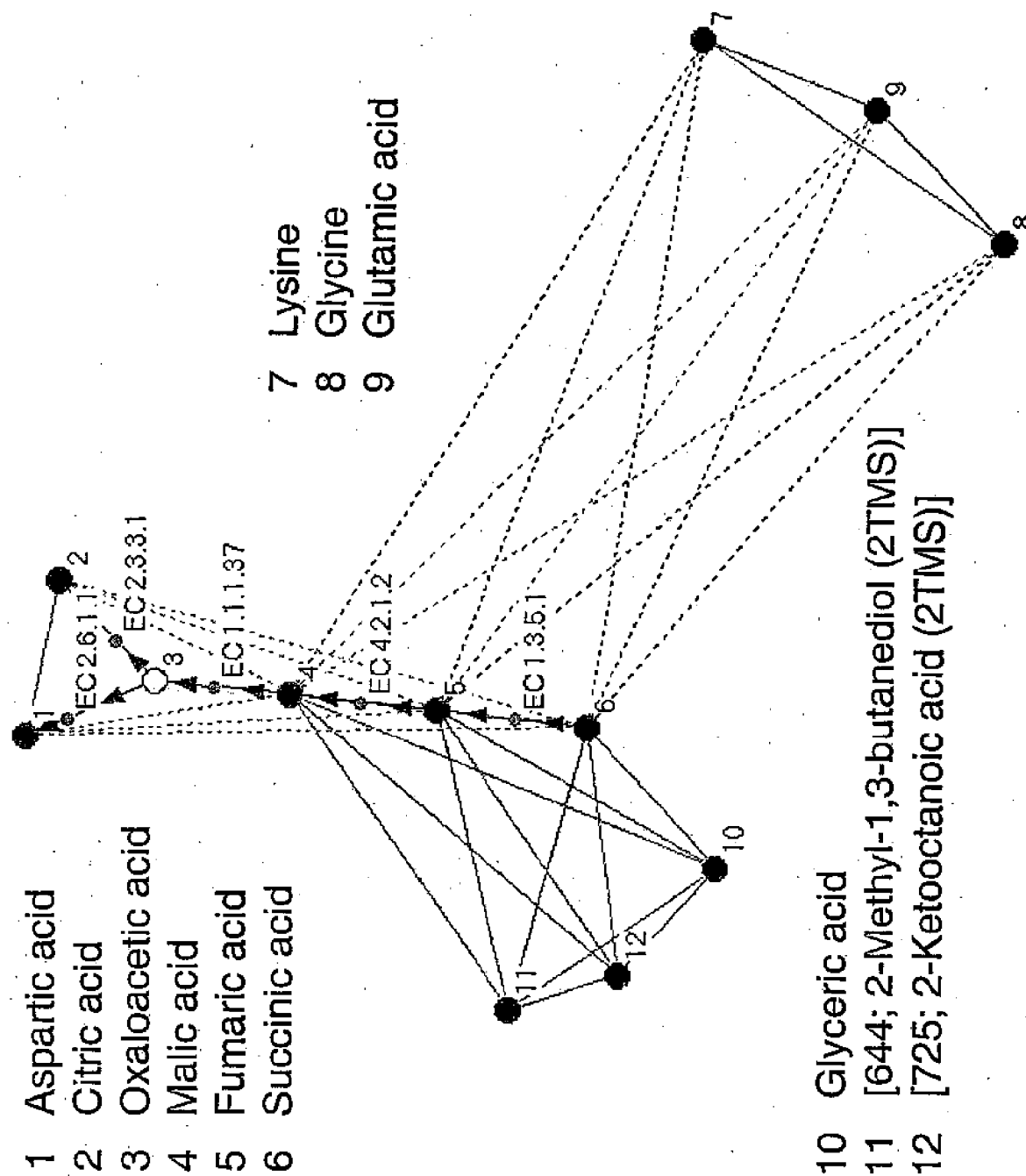
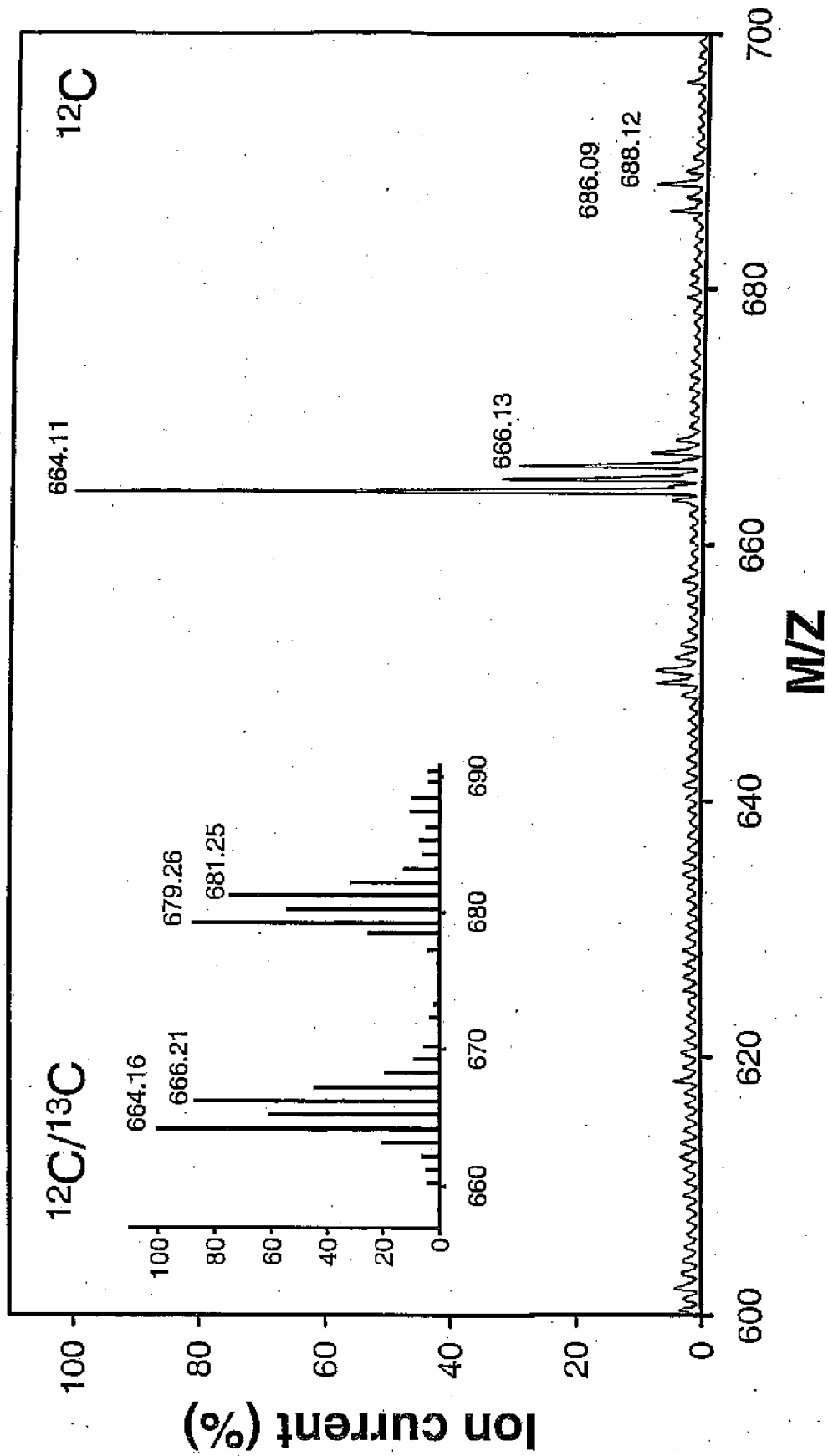


Figure 9



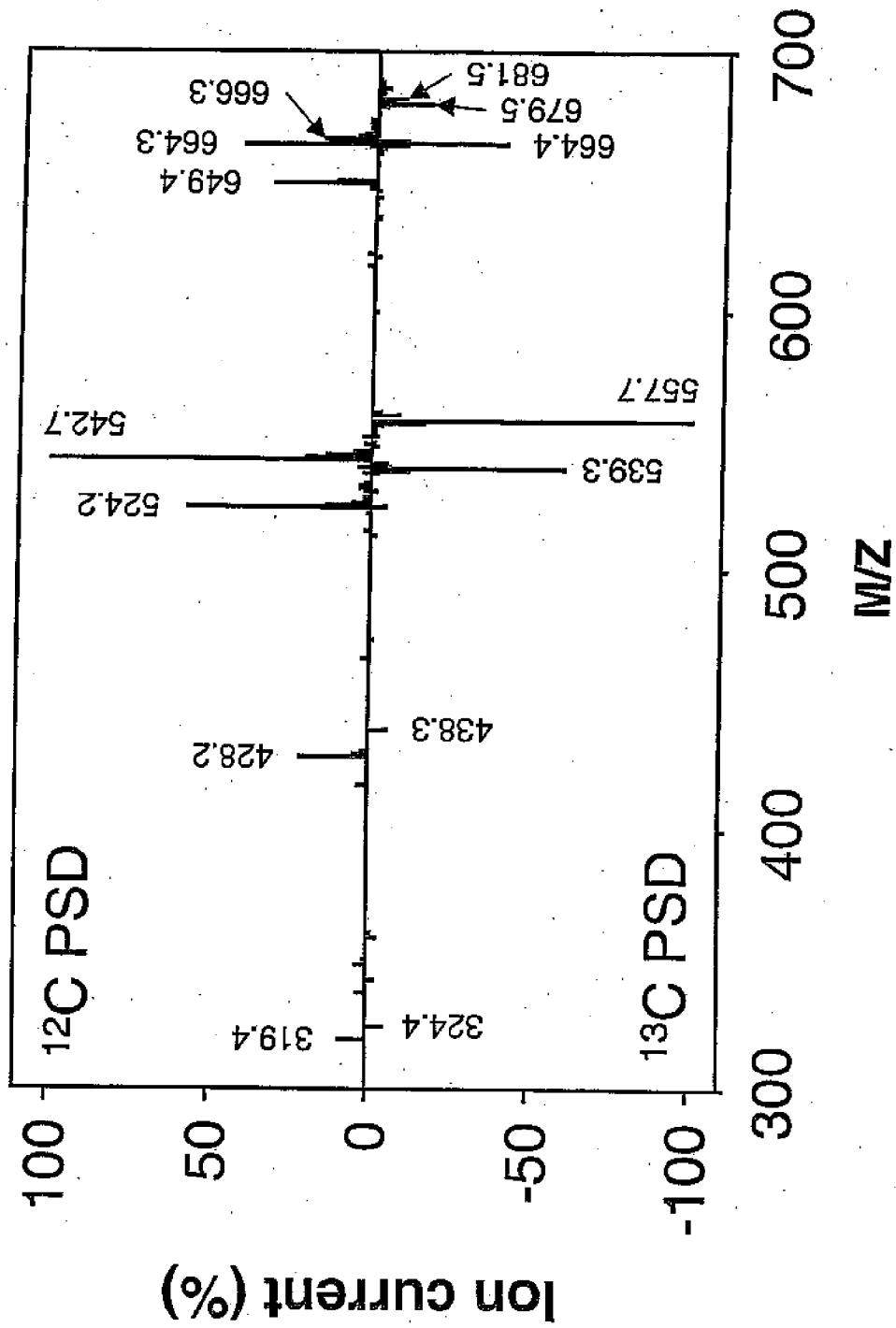


Figure 10